15 Esters

CONTENTS

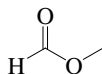## 15.1 LIST OF CHEMICALS AND DATA COMPILATIONS

15.1.1 ALIPHATIC ESTERS

15.1.1.1 Methyl formate

Common Name: Methyl formate
Synonym: formic acid methyl ester, methyl methanoate
Chemical Name: methyl formate
CAS Registry No: 107-31-3
Molecular Formula: $C_2H_4O_2$, $HCOOCH_3$
Molecular Weight: 60.052
Melting Point (°C):
    –99.0   (Weast 1982–83; Dean 1985; Lide 2003)
Boiling Point (°C):
    31.7   (Lide 2003)
Density (g/cm³ at 20°C):
    0.9742   (Weast 1982–83)
    0.9742, 0.9664   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    62.8   (exptl. at normal bp, Lee et al. 1972)
    61.6   (20°C, calculated-density)
    62.6   (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    30.59; 29.72   (25°C; bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.75   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    230000   (USEPA 1975; quoted, Howard 1993)
    304000   (20°C, Verschueren 1983)
    230000   (Dean 1985; Riddick et al. 1986)
    23800   (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    83260*   (isoteniscope method, measured range 21–31.7°C, Nelson 1928)
    log (P/mmHg) = 7.2202 – 1320.8/(T/K); temp range 21–31.7°C, Nelson 1928)
    53329*   (16°C, summary of literature data, temp range –74.2 to 213°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 7027.8/(T/K)] + 7.852144; temp range –74.2 to 213°C (Antoine eq., Weast 1972–73)
    63980, 93310   (20°C, 30°C, Verschueren 1983)
    80840   (calculated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 2.11093 – 1.573/(–17.263 + t/°C), temp range: 21–31.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    83440   (calculated-Antoine eq., Dean 1985)
    log (P/mmHg) = 3.207 – 3.02/(–11.9 + t/°C), temp range: 21–32°C (Antoine eq., Dean 1985, 1992)
    78060   (selected lit., Riddick et al. 1986)
    log (P/kPa) = 6.29529 – 1125.2/(174.2 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
    78600   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.225693 - 1088.955/(-46.675 + T/K)$; temp range 279–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log $(P_L/kPa) = 6.39684 - 1196.323/(-32.629 + T/K)$; temp range 305–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)

78070   (Daubert & Danner 1989)

log $(P/mmHg) = 28.9576 - 2.3582 \times 10^3/(T/K) - 7.4848 \cdot \log(T/K) + 7.4384 \times 10^{-10} \cdot (T/K) + 2.7013 \times 10^{-6} \cdot (T/K)^2$, temp range 174–487 K (vapor pressure eq., Yaws 1994)

114881   (35°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

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

22.61   (exptl., Hine & Mookerjee 1975)

20.15, 17.96   (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

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

26.02   (calculated-P/C, Hoff et al. 1993)

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

–0.010   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)

–0.264   (estimated, Howard 1993)

0.03   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

–0.222   (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

0.699   (soil, estimated-S, Lyman et al. 1990)

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

Volatilization: based on Henry's law constant, $t_{1/2} \sim 5.3$ h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

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

$k_{OH} = (2.27 \pm 0.34) \times 10^{-13}$ cm³ molecule^{-1} s^{-1} at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a, quoted, Atkinson 1989)

$k_{OH}(calc) = 0.43 \times 10^{-12}$ cm³ molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: aqueous base-catalyzed hydrolysis k = 36.6 M^{-1} s^{-1} at 25°C corresponds to $t_{1/2}$ = 21.9 d, 2.19 d, 9.1 h and 0.91 h at respective pHs of 6, 7, 8, and 9 (Mabey & Mill 1978; quoted, Howard 1993)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: estimated $t_{1/2}$ = 74 d, based on experimental reaction rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere at 23°C (Atkinson 1989; quoted, Howard 1993).

TABLE 15.1.1.1.1

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

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

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

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

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

Nelson 1928		Stull 1947	
isoteniscope		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
21.0	80101	−74.2	133.3
25.0	83260	−57.0	666.6
26.6	86286	−48.6	1333
26.8	87286	−39.2	2666
27.1	88392	−28.7	5333
28.3	90406	−21.9	7999
28.9	94845	−12.9	13332
30.1	96378	0.80	26664
31.4	101431	16.0	53329
31.7	102351	32.0	101325
bp/°C	31.6	mp/°C	−99.8
eq. 1	P/mmHg		
A	7.2203		
B	1329.8		

Methyl formate: vapor pressure vs. 1/T

◇ Nelson 1928
▢ Stull 1947
✕ Alderson et al. 2003

b.p. = 32.7 °C
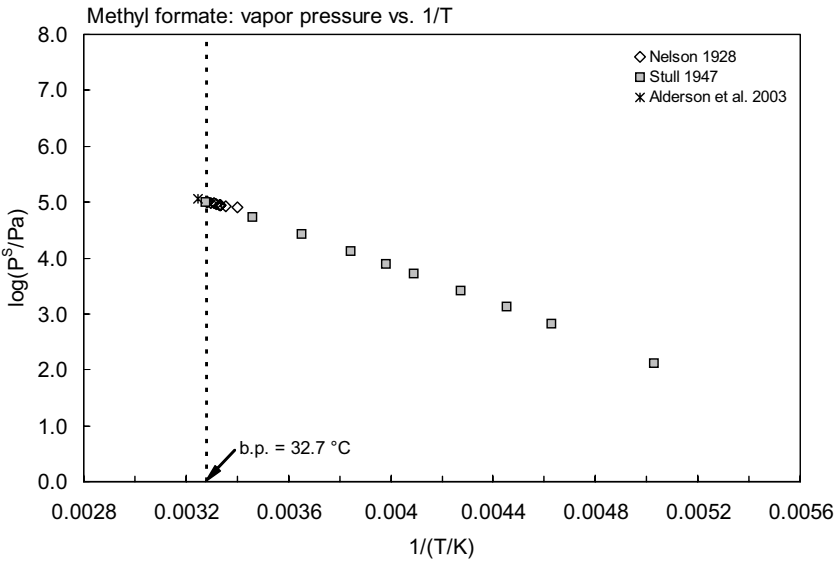
FIGURE 15.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methyl formate.

15.1.1.2   Ethyl formate
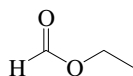
Common Name: Ethyl formate
Synonym: ethyl methanoate, formic acid ethyl ester
Chemical Name: ethyl formate
CAS Registry No: 109-94-4
Molecular Formula: $C_3H_6O_2$, $HCOOCH_2CH_3$
Molecular Weight: 74.079
Melting Point (°C):
    –79.6   (Lide 2003)
Boiling Point (°C):
    54.4   (Lide 2003)
Density (g/cm³ at 20°C):
    0.9168   (Weast 1982–83)
    0.9220, 0.9153   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    80.8   (20°C, calculated-density, Stephenson & Malanowski 1987)
    86.4   (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    31.64; 29.94   (25°C; bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.205   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    88250   (Seidell 1941)
    93260   (estimated, McGowan 1954)
    52440   (Deno & Berkheimer 1960)
    118000   (Verschueren 1983; Riddick et al. 1986)
    117000   (Dean 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    34530*   (25.4°C, isoteniscope method, measured range 25.4–55.4°C, Nelson 1928)
    log (P/mmHg) = 7.8457 – 1621.2/(T/K); temp range 25.4–55.4°C (Nelson 1928)
    33050*   (interpolated-regression of tabulated data, temp range –60.5 to 54.3°C, Stull 1947)
    30844*   (23.715°C, temp range 3.893–53.56°C, Mertl & Polak 1964 - ref. see Boublik et al. 1984)
    log (P/mmHg) = [–0.2185 × 7511.7/(T/K)] + 7.842747; temp range –60.5 to 225°C (Antoine eq., Weast 1972–73)
    25590, 39990   (20°C, 30°C, Verschueren 1983)
    30840, 32610   (23.7°C, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 6.13263 – 1123.305/(218.177 + t/°C); temp range 3.89–53.56°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    32540   (interpolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 7.0090 – 1123.94/(218.2 + t/°C); temp range 4–54°C (Antoine eq., Dean 1985, 1992)
    32370   (selected, Riddick et al. 1986)
    33070   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.1384 – 1151.08/[–48.94 + (T/K)]; temp range: 213–336 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 6.4206 – 1326.4/[–26.867 + (T/K)]; temp range: 327–498 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 29.9404 – 2.5263 × 10³/(T/K) – 7.809·log(T/K) – 1.0111 × 10⁻⁹·(T/K) + 2.7447 × 10⁻⁶·(T/K)²;
  temp range 194–508 K (vapor pressure eq., Yaws 1994)

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

28.46	(exptl., Hine & Mookerjee 1975)
27.18, 25.96	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
17.55	(calculated-MCI χ, Nirmalakhandan & Speece 1988)
702.0	(calculated, Hoff et al. 1993)

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

–0.38	(calculated, Iwasa et al. 1965)
0.23	(calculated, Hansch et al. 1968)
0.33	(Leo et al. 1971)
0.55	(calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)
0.26	(calculated-CLOGP, Müller & Klein 1992)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

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} = (10.2 ± 1.4) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted, Atkinson 1989)

  k_{OH} = 10.2 × 10⁻¹² cm³ molecule⁻¹ s⁻¹; k(soln) = 6.5 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

  k_{OH}(calc) = 1.17 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 15.1.1.2.1

Reported vapor pressures of ethyl formate 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)		

Nelson 1928		Stull 1947		Mertl & Polak 1964	
isoteniscope		summary of literature data		ref in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.4	34530	–60.5	133.3	3.893	11870
28.9	40103	–42.2	666.6	5.883	13155

(Continued)

TABLE 15.1.1.2.1 (*Continued*)

Nelson 1928		Stull 1947		Mertl & Polak 1964	
isoteniscope		summary of literature data		ref in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
33.6	48263	−33.0	1333	8.963	15369
35.5	51982	−22.7	2666	12.395	18244
38.2	58555	−11.5	5333	16.185	21869
40.1	61608	−4.30	7999	19.290	25242
42.9	70914	5.40	13332	23.715	30844
44.2	72304	20.0	26664	28.260	37517
47.8	82193	40.0	53329	32.775	45345
50.9	91886	53.4	101325	38.220	56435
52.2	96139			43.630	69674
53.4	100392	mp/°C	−79	49.453	86066
54.2	102978			53.560	99805
55.4	109138				
				eq. in Boublik et al. 1984	
bp/°C	53.8			eq. 2	P/kPa
				A	6.13263
eq. 1	P/mmHg			B	1123.305
A	7.8457			C	218.177
B	1621.6			bp/°C	54.013

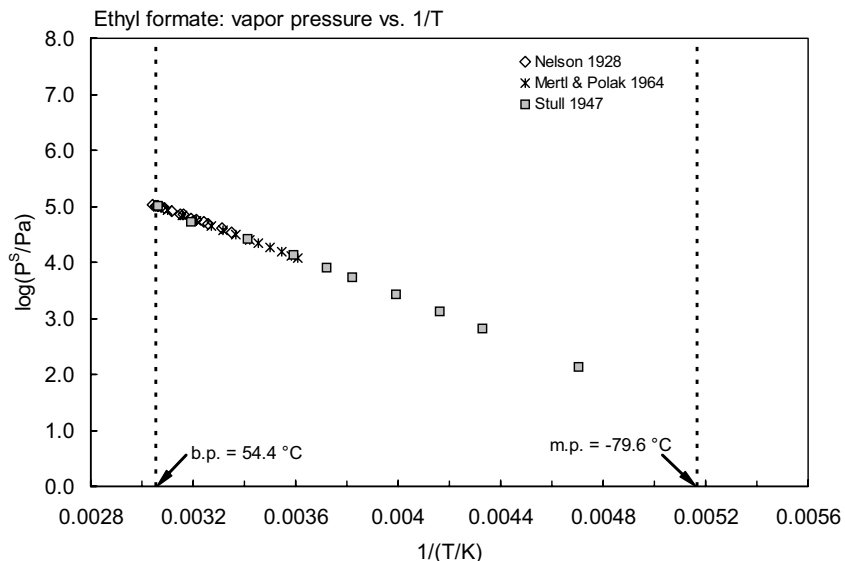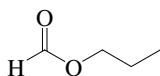Ethyl formate: vapor pressure vs. 1/T

FIGURE 15.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl formate.

15.1.1.3   Propyl formate

Common Name: Propyl formate
Synonym: formic acid propyl ester, methanoic acid *n*-propyl ester, propyl methanoate
Chemical Name: *n*-propyl formate, propyl formate
CAS Registry No: 110-74-7
Molecular Formula: $C_4H_8O_2$, $HCOOCH_2CH_2CH_3$
Molecular Weight: 88.10 6
Melting Point (°C):
   –92.9   (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
   80.9   (Lide 2003)
Density (g/cm³ at 20°C):
   0.9058   (Weast 1982–83)
   0.9006   (Dean 1985)
   0.9055, 0.8996   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
   97.3   (20°C, calculated-density)
   110.8   (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   37.49; 33.60   (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   28445   (Seidell 1941)
   27230   (Deno & Berkheimer 1960)
   27300   (Hansch et al. 1968; quoted, Hine & Mookerjee 1975; Müller & Klein 1992)
   20500   (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   11759*   (26.2°C, isoteniscope method, measured range 26.2–82.3°C, Nelson 1928)
   log (P/mmHg) = 7.9925 – 1806.5/(T/K); temp range 26.2–82.3°C (Nelson 1928)
   10620*   (interpolated-regression of tabulated data, temp range –43 to 81.3°C Stull 1947)
   log (P/mmHg) = [–0.2185 × 8208.1/(T/K)] + 7.891833; temp range –43 to 245°C (Antoine eq., Weast 1972–73)
   11010   (calculated-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 5.98912 – 1135.489/(204.518 + t/°C); temp range: 26.2–82.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   10710   (extrapolated-Antoine eq., Dean 1985)
   log (P/mmHg) = 6.848 – 1127/(203 + t/°C); temp range: 26–82°C (Antoine eq., Dean 1985, 1992)
   11030   (quoted lit. average, Riddick et al. 1986)
   log (P/kPa) = 5.97008 – 1132.3/(204.8 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
   10810   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
   log $(P_L$/kPa) = 6.73268 – 1560.69/(–24.287 + T/K); temp range: 230–335 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   log $(P_L$/kPa) = 6.2378 – 1301.3/(–46.767 + T/K); temp range: 354–518 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = $28.6983 - 2.6926 \times 10^3/(T/K) - 7.2435 \cdot \log(T/K) - 8.7226 \times 10^{-11} \cdot (T/K) + 1.9456 \times 10^{-6} \cdot (T/K)^2$; temp range 180–538 K (vapor pressure eq., Yaws 1994)

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

37.52 (exptl., Hine & Mookerjee 1975)
38.39, 38.39 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
22.61 (calculated-MCI χ, Nirmalakhandan & Speece 1988)

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

0.73 (calculated, Hansch et al. 1968)
0.83 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979)
0.83 (recommended, Sangster 1989; 1993)
0.83 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:
Photolysis:
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:
$k_{OH} = (2.38 \pm 2.7) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988; quoted, Atkinson 1989)
k_{OH}(calc) = 1.87×10^{-12} cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 15.1.1.3.1

Reported vapor pressures of propyl formate 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)		

n-propyl formate				isopropyl formate			
Nelson 1928		Stull 1947		Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data		isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
26.2	11759	–43.0	133.3	25.1	18198	–52.0	133.3
30.8	14545	–22.7	666.6	29.8	22585	–32.7	666.6
35.2	17932	–12.6	1333	35.0	28958	–22.7	1333
40.5	22718	–1.70	2666	41.2	37530	–12.1	2666

TABLE 15.1.1.3.1 (*Continued*)

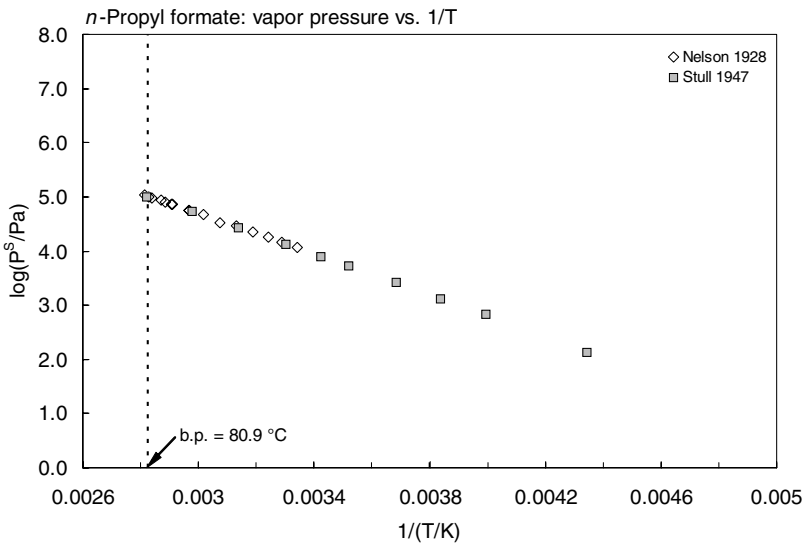| *n*-propyl formate				isopropyl formate			
Nelson 1928		Stull 1947		Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data		isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
46.2	28864	10.8	5333	48.0	49062	0.20	5333
52.0	33717	18.8	7999	48.2	49609	7.50	7999
58.4	46516	29.5	13332	53.708	61101	17.8	13332
63.7	56235	45.3	26664	57.80	70661	33.6	26664
63.9	57422	62.6	53329	63.90	87726	50.5	53329
70.5	72034	81.3	101325	68.60	102405	68.3	101325
71.0	73967			70.30	108377		
73.5	79993	mp/°C	−92.5	77.788	113830	mp/°C	-
75.1	86513			72.100	116430		
78.9	96525						
80.5	101245			bp/°C	68.4		
82.3	106498			eq. 1	P/mmHg		
				A	7.8909		
bp/°C	80.4			B	1710.5		
eq. 1	P/mmHg						
A	7.99255						
B	1806.5						

FIGURE 15.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-propyl formate.

15.1.1.4　Methyl acetate

Common Name: Methyl acetate
Synonym: acetic acid methyl ester, ethanoic acid methyl ester, methyl ethanoate
Chemical Name: methyl acetate
CAS Registry No: 79-20-9
Molecular Formula: $C_3H_6O_2$, CH_3COOCH_3
Molecular Weight: 74.079
Melting Point (°C):
　　–98.25　　　Lide 2003)
Boiling Point (°C):
　　56.89　　　(Lide 2003)
Density (g/cm³ at 20°C):
　　0.9330　　　　　(Weast 1982–83)
　　0.9342　　　　　(Dean 1985)
　　0.9342, 0.9279　　　(20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
　　79.3　　　(20°C, calculated-density)
　　84.8　　　(calculated-Le Bas method at normal boiling point)
Dissociation Constant:
　　22.50　　　(pK_s, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
　　32.30, 30.33　　　(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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
　　243730　　　(20°C, shake flask-turbidity, Fühner 1924)
　　294920　　　(estimated, McGowan 1954)
　　243500　　　(20°C, Stephen & Stephen 1963)
　　240000, 319000　　　(20°C, Verschueren 1983)
　　240000　　　(Dean 1985)
　　245000　　　(20°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
　　27980*　　　(interpolated-regression of tabulated data, –52 to 57.8°C, Stull 1947)
　　25242*　　　(22.060°C, temp range 1.758–55.840°C, Mertl & Polak 1964; quoted, Boublik et al. 1984)
　　log (P/mmHg) = [–0.2185 × 7732.8/(T/K)] + 7.938782; temp range –57.2 to 225°C (Antoine eq., Weast 1972–73)
　　28830*　　　(ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
　　log (P/kPa) = 6.24410 – 1183.700/(T/K) – 50.736; temp range 259.6–351.3 K (Antoine eq., ebulliometry, Ambrose et al. 1981)
　　31330　　　(Verschueren 1983)
　　28830　　　(interpolated-Antoine eq., Boublik et al. 1984)
　　log (P/kPa) = 6.25449 – 1189.608/(223.115 + t/°C); temp range –13.58 to 78.12°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
　　log (P/kPa) = 6.19357 – 1159.358/(219.913 + t/°C); temp range 1.76–55.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
　　28200　　　(calculated-Antoine eq., Dean 1985)
　　log (P/mmHg) = 7.0652 – 1157.63/(219.73 + t/°C); temp range: 1–56°C (Antoine eq., Dean 1985, 1992)
　　28828　　　(lit. average, Riddick et al. 1986)

log (P/kPa) = 6.24410 – 1183.70/(222.414 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

28830, 28840 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.190152 – 1157.622/(–53.426 + T/K); temp range 274–331 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.18771 – 1156.219/(–53.589 + T/K); temp range: 274–331 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 33.7235 – 2.7204 × 10³/(T/K) –9.1182·log(T/K) – 9.4316 × 10⁻¹¹·(T/K) + 3.3102 × 10⁻⁶·(T/K)²; temp range 175–507 K (vapor pressure eq., Yaws 1994)

53808 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):

9.190 (volatility-partial pressure, Butler & Ramchandani 1935)

11.65 (volatility-partial pressure-GC, Buttery et al. 1969)

8.795 (exptl., Hine & Mookerjee 1975)

11.59, 9.210 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

13.06 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 39.2 kJ/mol, Kieckbusch & King 1979)

9.210, 25.96 (quoted, calculated-MCI χ, Nirmalakhandan & Speece 1988)

9.80 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 4.590 – 2048/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.18 (shake flask-CR, Collander 1951; quoted, Hansch & Leo 1979; Hansch & Leo 1985)

0.23 (calculated, Hansch et al. 1968)

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

0.18 (recommended, Sangster 1989, 1993)

0.18 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

–0.224 (calculated-S, Lyman et al. 1982)

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

Sorption Partition Coefficient, log K_{OC}:

0.681 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)

1.474 (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)

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

Volatilization: based on calculated Henry's law constant, $t_{1/2}$ ~ 9.1 h from a model river of 1 m deep flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

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

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

k_{OH} = (1.1 ± 0.03) × 10¹⁰ dm³ mol⁻¹ s⁻¹ or (1.7 ± 0.5) × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 292 K using relative rate technique for *n*-butane (Campbell & Parkinson 1978)

k_{OH}(exptl) = (1.3 – 3.41) × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988a,b; quoted, Howard 1993)

k_{OH}(calc) = 1.9 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, k_{OH}(obs.) = 1.7 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1985)

k_{OH}(calc) = 2.2 × 10^{-13} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.7 × 10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

k_{OH} = (3.41 ± 0.29) × 10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K (absolute rate, flash photolysis-resonance fluorescence, Wallington 1988a)

k_{OH} = 3.41 × 10^{-13} cm^3 molecule^{-1} s^{-1}; k(soln) = 2.0 × 10^{-13} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

k_{OH}(calc) = 6.9 × 10^{-13} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant k = 0.182 M^{-1} s^{-1} at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

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

atmospheric $t_{1/2}$ = 47–94 d, based on exptl. rate constants for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.1.4.1

Reported vapor pressures of methyl acetate 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		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		ref. in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–57.2	133.3	1.758	9202	–13.581	3785	57.559	103841
–38.6	666.6	4.058	10415	–10.401	4597	61.773	119919
–29.3	1333	6.568	11870	–7.621	5426	65.575	136076
–19.1	2666	8.563	13155	–4.400	6450	70.114	157575
–7.90	5333	11.635	15369	–1.427	7733	74.442	180470
–0.50	7999	15.145	18244	1.819	9241	78.128	202007
9.40	13332	18.975	21869	4.978	10938	25.0	28828
24.0	26664	22.060	25242	8.278	12977		
40.0	53329	26.520	30844	11.635	15386	bp/K	330.018
57.8	101325	31.060	37517	14.886	18029		
		35.590	45345	19.151	22079	Antoine eq.	
mp/°C	–98.7	41.090	56435	22.787	26098	eq. 3	P/kPa
		46.500	69474	26.948	31418	A	6.24410
		52.310	86066	31.023	37456	B	1184.700
		55.840	97512	35.319	44810	C	–50.735

TABLE 15.1.1.4.1 (*Continued*)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		ref. in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				40.047	54206		
				44.148	63603	data also fitted to:	
				48.507	74964	Chebyshev equation and	
				53.215	89039	Chebyshev polynomial	
				56.821	101164	coefficients given in ref.	

FIGURE 15.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for methyl acetate.

15.1.1.5 Vinyl acetate
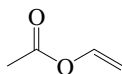
Common Name: Vinyl acetate
Synonym: ethanoic acid ester, ethenyl acetate, ethenyl ethanoate
Chemical Name: ethenyl acetate, vinyl acetate
CAS Registry No: 108-05-4
Molecular Formula: $C_4H_6O_2$, $CH_3COOCH=CH_2$
Molecular Weight: 86.090
Melting Point (°C):
   –93.2   (Weast 1982–83: Lide 2003)
Boiling Point (°C):
   72.8   (Lide 2003)
Density (g/cm^3 at 20°C):
   0.9317   (Weast 1982–83)
Molar Volume (cm^3/mol):
   92.2   (20°C, calculated-density, Stephenson & Malanowski 1987)
   101.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   37.2, 34.35 (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
   19722   (Deno & Berkheimer 1960)
   25000   (Verschueren 1983)
   20000   (Dean 1985)
   20000   (20°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   14454*   (interpolated-regression of tabulated data, temp range –48 to 72.5°C, Stull 1947)
   21.83*   (21.83°C, measured range 21.8–72.04°C, Capkova & Fried 1964 - ref see Boublik et al. 1984)
   84406*   (67°C, vapor-liquid equilibrium data, measured range 67–82°C, Swamy & Van Winkle 1965)
   15300   (interpolated-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 7.17023 – 1766.918/(269.951 + t/°C); temp range: 67–82°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   log (P/kPa) = 6.3363 – 1296.847/(226.731 + t/°C); temp range: 21.83–72.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
   15300   (interpolated-Antoine eq., Dean 1985, 1992)
   log (P/mmHg) = 7.2101 – 1296.13/(226.66 + t/°C); temp range: 22–72°C (Antoine eq., Dean 1985, 1992)
   14100   (quoted lit. average, Riddick et al. 1986)
   log (P/kPa) = 7.216 – 1798.4/(T/K); temp range: not specified (Antoine eq., Riddick et al. 1986)
   15340, 15305   (interpolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
   log (P_L/kPa) = 6.3799 – 1320.2716/(–43.96 + T/K); temp range: 293–346 K (Antoine eq.-I, Stephenson & Malanowski 1987)
   log (P_L/kPa) = 6.34264 – 1300.315/(–46.041 + T/K); temp range 294–346 K (Antoine eq.-II, Stephenson & Malanowski 1987)
   11320   (20°C, quoted, Howard 1989)

log $(P/mmHg) = 12.722 - 2.177 \times 10^3/(T/K) - 91.458 \cdot \log (T/K) - 4.5688 \times 10^{-3} \cdot (T/K) + 2.9673 \times 10^{-6} \cdot (T/K)^2$;
temp range 180–524 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
48.74   (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW}:
0.60   (shake flask, Fujisawa & Masuhara 1980)
0.21   (calculated-HPLC-RT, Fujisawa & Masuhara 1981)
0.73   (recommended, Sangster 1989, 1993)
0.73   (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.32–0.37   (estimated-K_{OW}, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
1.28–1.77   (estimated-K_{OW}, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2}$ = 4.4 h from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{1/2}$ = 2.2 d from an environmental pond (Howard 1989).
Photolysis:
Oxidation: $t_{1/2}$ = 13 and 8 d for reactions with OH radical and singlet oxygen in sunlit natural water (Howard 1989).
Hydrolysis: overall rate constant $k_h = 1.10 \times 10^{-6}$ s^{-1} with $t_{1/2}$ = 7.3 d at 25°C and pH 7 (Mabey & Mill 1978) degradation $t_{1/2}$ = 7.3 d at 25°C and pH 7, the hydrolysis rate will increase as the pH increases (Howard 1989).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: estimated $t_{1/2}$ = 12 h with photochemically produced hydroxyl radical in an average atmosphere (Howard 1989).
Surface water: hydrolysis degradation $t_{1/2}$ = 7.3 days at 25°C and pH 7; $t_{1/2}$ = 13 and 8 d for reactions with hydroxyl radical and singlet oxygen, respectively, in natural water (Howard 1989).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 15.1.1.5.1
Reported vapor pressures of vinyl acetate 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		Capkova & Fried 1963		Swamy & Van Winkle 1965	
summary of literature data		in Boublik et al. 1984		V–L equil. data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–48.0	133.3	21.83	13159	67.0	84406
–28.0	666.6	25.12	15372	69.0	90646
–18.0	1333	28.8	18252	70.0	92899
–7.0	2666	32.85	21891	72.0	100711
5.30	5333	36.13	25264	74.0	107924
13.0	7999	40.82	30864	76.0	115550
23.3	13332	45.64	37543	78.0	123643
38.4	26664	50.37	45356	80.0	132189
55.5	53329	56.12	56448	82.0	131215
72.5	101325	61.83	69487		
		67.92	86046		
mp/°C	–73	72.04	99958		
		eq. 2	P/kPa		
		A	6.33630		
		B	1296.847		
		C	226.731		
		bp/°C	71.731		
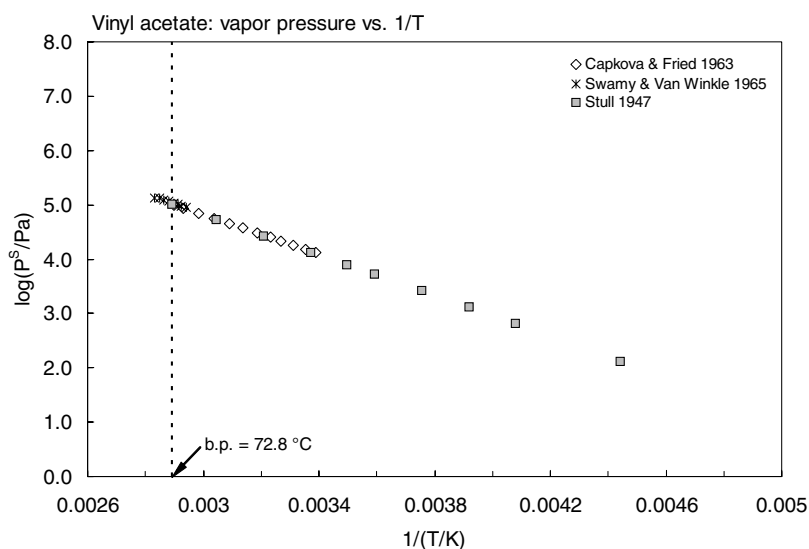
FIGURE 15.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for vinyl acetate.

15.1.1.6 Ethyl acetate
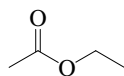
Common Name: Ethyl acetate
Synonym: acetic acid ethyl ester, acetic ether, ethanoic acid ester, ethyl ethanoate
Chemical Name: *n*-ethyl acetate, ethyl acetate
CAS Registry No: 141-78-6
Molecular Formula: $C_4H_8O_2$, $CH_3COOCH_2CH_3$
Molecular Weight: 88.106
Melting Point (°C):
    –83.8   (Lide 2003)
Boiling Point (°C):
    77.11   (Lide 2003)
Density (g/cm³ at 20°C):
    0.9003   (Weast 1982–83)
    0.9006, 0.8946   (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    106.0   (exptl. at normal bp, Lee et al. 1972)
    97.8   (20°C, calculated-density)
    108.6   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    22.83   (pK$_s$, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    35.62, 31.97 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    10.50   (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    64408   (20°C, shake flask-turbidity, Führer 1924)
    85300   (20°C, synthetic method, Jones 1929)
    78720   (shake flask-centrifuge, Booth & Everson 1948)
    80100*   (turbidimetric method, measured range 20–40°C, Altshuller & Everson 1953)
    80400*   (average, Altshuller & Everson 1953)
    79780   (shake flask-interferometry, Donahue & Bartell 1952)
    69990   (estimated, McGowan 1954)
    82220   (Deno & Berkheimer 1960)
    80350   (shake flask-UV, Hansch et al. 1968)
    63960   (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
    82500, 74000   (20°C, 35°C, literature average, Verschueren 1983)
    80000   (shake flask-HPLC, Banerjee 1984)
    97000   (Dean 1985)
    95000   (shake flask-radiometric method, Lo et al. 1986)
    80800   (lit. average, Riddick et al. 1986)
    77900*   (20.2°C, shake flask-GC/TC, measured range 0–70°C, Stephenson & Stuart 1986)
    73700   (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    13330*, 11860   (27.0°C, interpolated-regression of tabulated data, temp range –43.4 to 78.1°C, Stull 1947)
    log (P/mmHg) = 7.30588 – 1357.7/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

13155*   (25.86°C, temp range 15.58–75.830°C, Mertl & Polak 1964; quoted, Boublik et al. 1984)

log (P/mmHg) = [–0.2185 × 8301.1/(T/K)] + 8.001170; temp range –43.4 to 235°C (Antoine eq., Weast 1972–73)

12600*   (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

log (P/kPa) = 6.18799 – 1224.673/(T/K) – 57.438; temp range: 271–372.865 K (Antoine eq., ebulliometry, Ambrose et al. 1981)

9704   (20°C, Verschueren 1983)

11220   (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.1171 – 1245.172/(217.984 + t/°C), temp range 15.58–75.83°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.20229 – 1232.542/(216.587 + t/°C), temp range –2.08 to 99.71°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

12620   (calculated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.10179 – 1244.95/(217.88 + t/°C) temp range 15–76°C (Antoine eq., Dean 1985, 1992)

12600   (lit. average, Riddick et al. 1986)

log (P/kPa) = 6.18799 – 1224.673/(215.712 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

12620   (interpolated-Antoine eq.-I and III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.227229 – 1245.239/(–55.239 + T/K); temp range: 288–351 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.38462 – 1369.41/(–37.675 + T/K); temp range: 350–508 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.22825 – 1245.68/(–55.193 + T/K); temp range: 288–351 K (Antoine eq.-III, Stephenson & Malanowski 1987)

3240, 5240 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = 0.6955 – 2.2498 × 10^3/(T/K) + 5.4643·log(T/K) – 1.9451 × 10^{-2}·(T/K) + 1.2362 × 10^{-5}·(T/K)^2; temp range 190–623 K (vapor pressure eq., Yaws 1994)

25078   (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 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):

13.42   (partial pressure, Butler & Ramchandani 1935)

17.78   (28°C, concn. ratio-GC, Nelson & Hoff 1968)

13.62   (exptl., Hine & Mookerjee 1975)

15.64, 13.94 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

17.20   (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 41.4 kJ/mol, Kieckbusch & King 1979)

13.62, 24.22 (quoted, calculated-MCI χ, Nirmalakhandan & Speece 1988)

41.72*   (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

ln (1/K_{AW}) = –7.28 + 3563/(T/K), temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)

13.62, 6.23 (quoted, calculated-molecular structure, Russell et al. 1992)

11.33   (calculated, Hoff et al. 1993)

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

12.72   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 5.095 – 2163/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.66   (shake flask-chemical reaction CR, Collander 1951)

0.73   (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1969, 1971; Hansch & Leo 1979)

0.73   (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979)

0.65, 0.66 (calculated-π substituent const.; calculated-fragment const., Rekker 1977)

0.70   (exptl., Valvani et al. 1981; quoted, Amidon & Williams 1982)

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

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

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

0.73   (recommended, Sangster 1989, 1993)

0.73   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

    4.13   (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
    0.70   (alga *Chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)
    1.48   (golden ide, Freitag et al. 1985)
    4.13   (algae, Freitag et al. 1985)
    3.52   (activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

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

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

    Volatilization: using Henry's law constant, $t_{\frac{1}{2}} \sim 10.1$ h was estimated for a model river of 1 m deep flowing at
        1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).
    Photolysis: rate constant $k = 6.8 \times 10^{-4}$ h^{-1} to 2.21×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution
        and with HO- in the gas (Dilling et al. 1988).
    Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
        with NO$_3$ radical and k_{O3} with O$_3$ or as indicated, *data at other temperatures and/or Arrhenius equation
        see reference:
        photooxidation $t_{\frac{1}{2}} = 2.75–110$ yr in water, based on measured rate constant for the reaction with hydroxyl
            radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)
        photooxidation $t_{\frac{1}{2}} = 2.4–24$ h for the gas-phase reaction with OH radical in air, based on the rate of
            disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
        $k_{OH} = (1.16 \pm 0.13) \times 10^9$ dm^3 mol^{-1} s^{-1} at 292 K using relative rate technique for *n*-butane (Campbell &
            Parkinson 1978)
        k_{OH}(calc) $= 1.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) $= 1.82 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp.
            (SAR structure-activity relationship, Atkinson 1985)
        k_{OH}(calc) $= 1.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) $= 1.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp.
            (SAR structure-activity relationship, Atkinson 1987)
        k_{OH}* $= (15.1 \pm 1.4) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K, measured range 296–440 K (flash photolysis-
            resonance fluorescence, Wallington et al. 1988a; quoted Atkinson 1989)
        $k_{OH} = 1.51 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}; k(soln) $= 6.6 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} for reaction with OH radical
            in aqueous solution (Wallington et al. 1988b)
        $k_{OH} = 1.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
        k_{OH}(calc) $= 1.94 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)
    Hydrolysis: alkaline hydrolysis rate constant $k = 0.110$ M^{-1} s^{-1} at 25°C in water (Salmi & Leimu 1947; quoted,
        Drossman et al. 1988);
        overall rate constant $k_h = 1.10 \times 10^{-8}$ s^{-1} with $t_{\frac{1}{2}} = 2.0$ yr at 25°C and pH 7 (Mabey & Mill 1978)
        $t_{\frac{1}{2}} = 2.02$ yr, based on measured rate constants for acid and base catalyzed and neutral hydrolysis at pH 7
            and 20°C (Mabey & Mill 1978; quoted, Howard 1990; Howard et al. 1991; Kollig 1993)
        $t_{\frac{1}{2}} = 9.5 \times 10^7$ d at pH 2, $t_{\frac{1}{2}} = 740$ d at pH 7 and $t_{\frac{1}{2}} = 97000$ d at pH 12 in natural waters at 20–25°C (Capel &
            Larson 1995)
    Biodegradation: aqueous aerobic $t_{\frac{1}{2}} = 24–168$ h, based on unacclimated aqueous aerobic biodegradation screening
        test data (Heukelekian & Rand 1955; Price et al. 1974; selected, Howard et al. 1991); aqueous anaerobic
        $t_{\frac{1}{2}} = 96–672$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
        $t_{\frac{1}{2}}$(aerobic) $= 1$ d, $t_{\frac{1}{2}}$(anaerobic) $= 4$ d in natural waters (Capel & Larson 1995)
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

    Air: photooxidation $t_{\frac{1}{2}} = 2.75 –110$ yr, based on measured rate constant for the reaction with OH radical in water
        (Dorfman & Adams 1973; selected, Howard et al. 1991);

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

photodecomposition $t_{1/2}$ = 14.6 h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

photooxidation $t_{1/2}$ = 35.3–353 h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991);

calculated lifetimes of 6.9 d and 10 yr for reactions with OH radical, NO₃ radical, respectively (Atkinson 2000).

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

Biodegradation $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 4 d; hydrolysis $t_{1/2}$ = 9.5×10^7 d at pH 2, $t_{1/2}$ = 740 d at pH 7 and $t_{1/2}$ = 97000 d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

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

Sediment:

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

Biota:

TABLE 15.1.1.6.1

Reported aqueous solubilities and Henry's law constants of ethyl acetate at various temperatures

Aqueous solubility				Henry's law constant	
Altshuller & Everson 1953		Stephenson & Stuart 1986		Kolb et al. 1992	
synthetic method-turbidity		shake flask-GC/TC		equilibrium headspace-GC	
t/°C	S/g·m⁻³	t/°C	S/g·m⁻³	t/°C	H/(Pa·m³ mol⁻¹)
20	83200	0	97100	40	41.72
25	80100	9.5	86200	60	94.53
30	77000	20.0	77900	70	130.9
35	73900	30.0	68100	80	167.8
40	70800	40.0	62800		
		50.0	62000	ln (1/K_{AW}) = A – B/(T/K)	
eq.	S/(g/100g)	59.9	60600	A	–7.28
S = 9.552 – 0.0618·(t/°C)		70.5	58800	B	–3563
summary of lit. average					
20	84200				
25	80400				
30	77000				
35	73900				
40	71200				
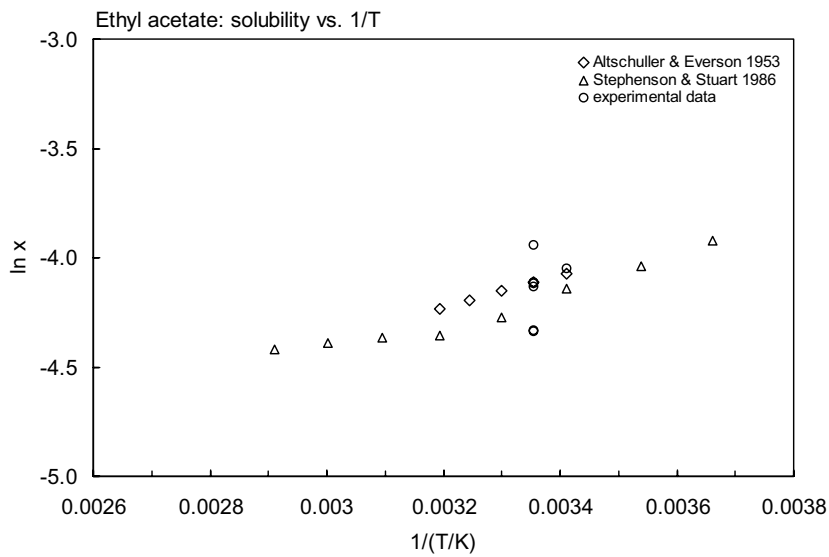
FIGURE 15.1.1.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for ethyl acetate.

TABLE 15.1.1.6.2
Reported vapor pressures of ethyl acetate 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		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−43.4	133.3	15.58	7838	−2.07	2868	29.112	15339
−23.5	666.6	18.58	9202	−0.096	3236	32.553	17990
−13.5	1333	21.115	10415	2.398	3754	37.060	22031
−3.0	2666	23.775	11870	5.737	4560	40.920	26056
9.10	5333	25.86	13155	8.692	5385	45.333	31374
16.6	7999	29.135	15369	12.098	6494	49.657	37046
27.0	13332	32.830	18244	15.242	7683	54.214	44760
42.0	26664	36.875	21869	18.681	9187	59.231	54168
59.3	53329	40.175	25242	22.022	10878	63.588	63565
77.1	101325	44.905	30844	25.532	12925	68.218	74938
		49.715	37517	29.119	15336	73.224	89016
mp/°C	−82.4	54.505	45345	32.599	17990	77.056	101144
		60.320	56435	37.086	22033	77.053	103823
		66.045	69474	40.929	26056	82.321	119902
		72.190	86066	25.0	12600	86.359	136066
		75.830	97272			91.183	157571
				bp/K	350.261	95.786	180471
		eq. 2	P/kPa			99.715	202018
		A	6.22710	Antoine eq.			

TABLE 15.1.1.6.2 (*Continued*)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1245.172	eq. 3	P/kPa	data also fitted to:	
		C	217.904	A	6.18799	Chebyshev equation and	
		bp	77.064	B	1224.673	Chebyshev polynomial	
				C	−57.438	coefficients given in ref.	
						bp/°C	77.115
						Bublik	P/kPa
						A	6.20229
						B	1232.542
						C	216.587

Ethyl acetate: vapor pressure vs. 1/T

◇ Mertl & Polak 1965
✻ Ambrose et al. 1981
▫ Stull 1947
△ Alderson et al. 2003
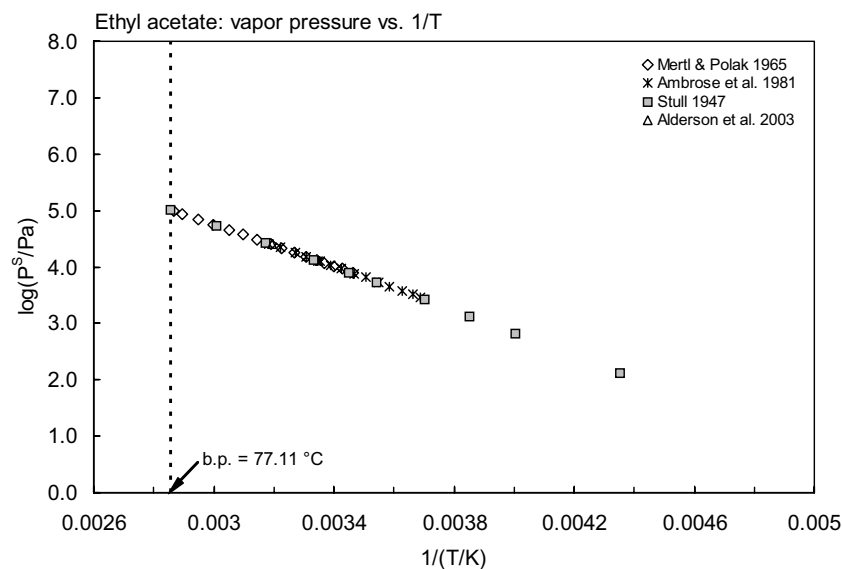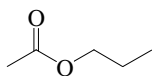
b.p. = 77.11 °C

FIGURE 15.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for ethyl acetate.

15.1.1.7 Propyl acetate

Common Name: Propyl acetate
Synonym: acetic acid propyl ester, propyl ethanoate, *n*-propyl acetate
Chemical Name: propyl acetate, *n*-propyl acetate
CAS Registry No: 109-60-4
Molecular Formula: $C_5H_{10}O_2$, $CH_3COOCH_2CH_2CH_3$
Molecular Weight: 102.132
Melting Point (°C):
    –93   (Lide 2003)
Boiling Point (°C):
    101.54   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8878   (Weast 1982–83)
    0.8830   (25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
    115.0   (20°C, calculated-density)
    133.0   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
    –7.18   (Perrin 1972)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    39.83, 33.86 (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperature designated * are compiled at the end of this section):
    18895   (20°C, shake flask-turbidity, Fühner 1924)
    18890   (Fühner 1924; quoted, Hansch et al. 1968)
    20380   (estimated, McGowan 1954)
    18160   (quoted, Deno & Berkheimer 1960)
    18900   (Stephen & Stephen 1963; quoted, Howard 1993)
    18895   (shake flask-UV, Hansch et al. 1968)
    20430   (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
    22450   (20°C, literature average, Verschueren 1983)
    23000   (Dean 1985)
    23000   (20°C, lit. average, Riddick et al. 1986)
    22600*, 19800   (20°C, 30°C, shake flask-GC/TC, measured range 0–90.2°C, Stephenson & Stuart 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    4152*   (interpolated-regression of tabulated data, temp range –26.7 to 101.8°C Stull 1947)
    $\log (P/mmHg) = [-0.2185 \times 8794.8/(T/K)] + 8.212268$; temp range –38.3 to 89°C (Antoine eq., Weast 1972–73)
    4478   (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
    $\log (P/kPa) = 6.14362 - 1284.080/(T/K) - 64.364$; temp range 290.3–398.908 K (Antoine eq., ebulliometry, Ambrose et al. 1981)
    4494   (interpolated-Antoine eq., Boublik et al. 1984)
    $\log (P/kPa) = 6.16547 - 1297.186/(210.301 + t/°C)$;. temp range 17.13–125.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    $\log (P/kPa) = 6.14152 - 1282.545/(208.628 + t/°C)$; temp range 39.8–100.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4486   (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.01615 – 1282.28/(208.6 + t/°C), temp range: 39–101°C (Antoine eq., Dean 1985, 1992)

4497   (quoted lit average, Riddick et al. 1986)

log (P/kPa) = 6.14362 – 1284.080/(208.786 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P$_L$/kPa) = 6.142106 – 1282.873/(–64.486 + T/K); temp range 312–374 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.48937 – 1544.31/(–30.623 + T/K); temp range 374–542 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P$_L$/kPa) = 6.13951 – 1281.682/(–64.58 + T/K); temp range 312–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/mmHg) = 43.0548 – 3.4692 × 10^3/(T/K) –12.217·log(T/K) + 2.4748 × 10^{-10}·(T/K) + 3.7508 × 10^{-6}·(T/K)^2; temp range 178–549 K (vapor pressure eq., Yaws et al. 1994)

9586   (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):

20.150   (exptl., Hine & Mookerjee 1975)

22.092, 20.62   (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

22.09   (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C, data presented in graph, ΔH = 43.2 kJ/mol, Kieckbusch & King 1979)

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

82.91, 203.7, 290.5, 387.3   (40, 60, 70 80°C, equilibrium headspace-GC, Kolb et al. 1992)

ln (1/K$_{AW}$) = –9.27 + 3971/(T/K), temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)

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

16.13   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K$_{AW}$ = 5.519 – 2257/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.23   (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)

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

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

1.23   (Hansch & Leo 1985)

1.24   (recommended, Sangster 1989. 1993)

1.24   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.380, 0.708 (calculated-S, calculated-K$_{OW}$, Lyman et al. 1982; quoted, Howard 1993)

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

1.288, 2.045 (soil, calculated-S, calculated-K$_{OW}$, Lyman et al. 1982; quoted, Howard 1993)

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

Volatilization: based on Henry's law constant, t$_{½}$ ~ 6.5 h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

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:

exptl. photooxidation rate constant of 2.4 to 4.1 × 10^{-12} cm³ molecule^{-1} s^{-1} for the vapor-phase reaction with the photochemically produced hydroxyl radicals in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993)

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

$k_{OH} = 4.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 305 ± 2 K using relative rate technique for 2-methylpropene (Winer et al. 1977; quoted, Atkinson 1985)

$k_{OH} = (1.7 \pm 0.2) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 296 K (Zetzsch 1982; quoted, Atkinson 1985)

k_{OH}(calc) = 2.7×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 4.2×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1985)

k_{OH}(calc) = 2.9×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 2.51×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (34.5 \pm 3.4) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 3.45 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}; k(soln) = 2.3×10^{-12} cm^3 molecule^{-1} s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 3.4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH}(calc) = 2.54×10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant k = 0.087 M^{-1} s^{-1} at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

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

t$_{1/2}$ = 3.39–6.69 d, based on exptl. rate constant for the vapor-phase reaction with the photochemically produced hydroxyl radical in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993).

TABLE 15.1.1.7.1
Reported aqueous solubilities of propyl acetate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	S/g·m^{-3}
0	32100
9.5	27800
20.0	22600
30.0	19800
40.0	18700
50.0	17200
60.1	16400
70.5	17200
80.0	16600
90.2	13500
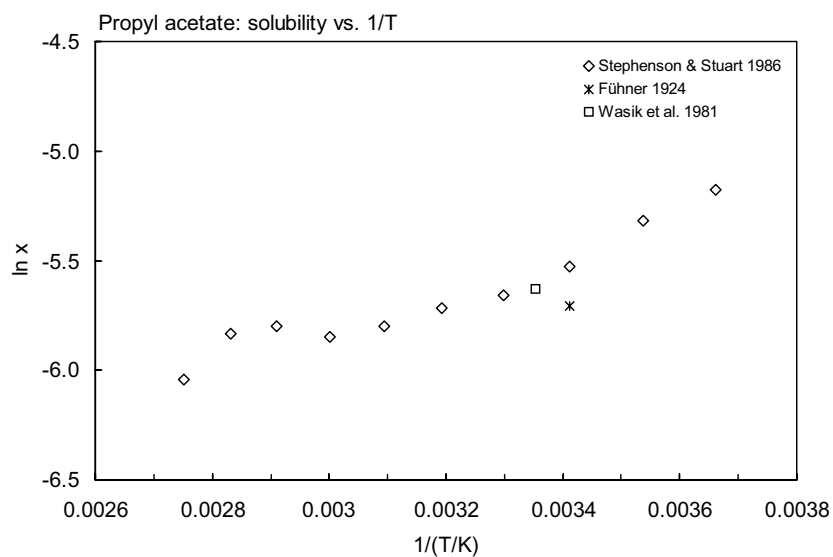
FIGURE 15.1.1.7.1 Logarithm of mole fraction solubility (In x) versus reciprocal temperature for propyl acetate.

TABLE 15.1.1.7.2
Reported vapor pressures of propyl acetate at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
–26.7	133.3
–5.40	666.6
5.0	1333
16.0	2666
28.8	5333
37.0	7999
47.8	13332
64.0	26664
82.0	53329
101.8	101325
mp/°C	–92.5
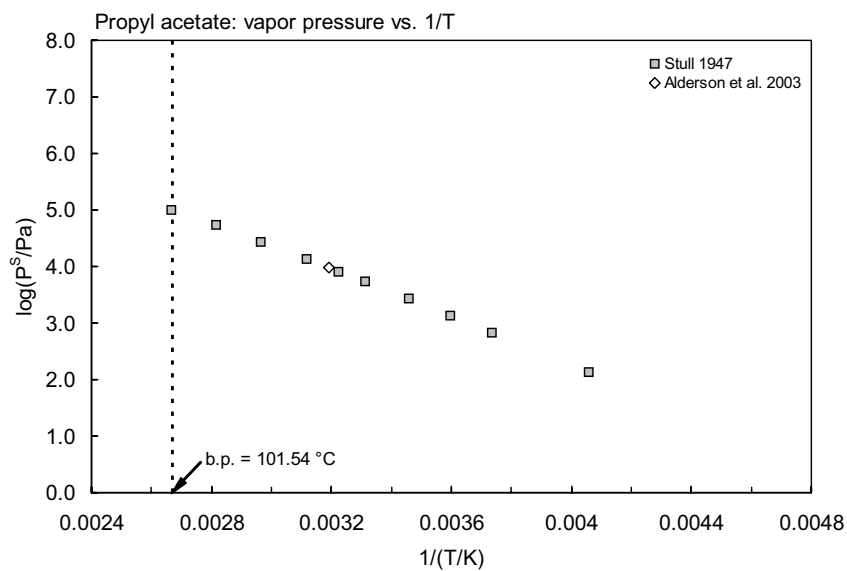
FIGURE 15.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for propyl acetate.

15.1.1.8   Butyl acetate
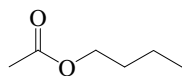
Common Name: Butyl acetate
Synonym: acetic acid butyl ester, butyl ethanoate, *n*-butyl acetate, ethanoic acid butyl ester
Chemical Name: butyl acetate, *n*-butyl acetate
CAS Registry No: 123-86-4
Molecular Formula: $C_6H_{12}O_2$, $CH_3COOCH_2CH_2CH_2CH_3$
Molecular Weight: 116.158
Melting Point (°C):
    –78   (Lide 2003)
Boiling Point (°C):
    126.1   (Lide 2003)
Density (g/cm³ at 20°C):
    0.8825   (Weast 1982–83)
    0.8764   (Riddick et al. 1986)
Molar Volume (cm³/mol):
    132.5   (20°C, calculated-density)
    155.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
    23.28   (pK_s, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    43.64, 35.81 (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    23550   (Seidell 1941)
    23180   (estimated, McGowan 1954)
    4955   (Deno & Berkheimer 1960)
    23580   (shake flask-spectrophotometry, Hansch et al. 1968)
    7040   (20°C, quoted, Amidon et al. 1975)
    6702   (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
    3936   (Hine & Mookerjee 1975)
    5000, 14000 (Verschueren 1983)
    4300   (Dean 1985)
    8400   (shake flask-radiometric method, Lo et al. 1986)
    6800   (20°C, quoted lit. average, Riddick et al. 1986)
    6400*, 5200 (19.7°C, 30.3°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson & Stuart 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
    designated * are compiled at the end of this section):
    log (P/mmHg) = 8.099 – 1964/(253 + t/°C) (Davis 1941)
    1560*   (24.5°C, measured range 24.5–94.1°C, Usanovich & Dembicij 1959)
    9210*   (59.74°C, temp range 59.74–126.09°C, Kliment et al. 1964; quoted, Boublik et al. 1984)
    3386*   (67.9°C, ebulliometry, measured range 67.9–124.0°C, Sheehan & Langer 1969)
    1505   (Hoy 1970)
    log (P/mmHg) = 6.9688 – 1326.7/(199.2 + t/°C); temp range 67.0–130°C (ebulliometry, Sheehan & Langer 1969)
    log (P/mmHg) = [–0.2185 × 9300.8/(T/K)] + 8.095046; temp range –21.2 to 118°C (Antoine eq., Weast 1972–73)
    1440   (quoted, Hine & Mookerjee 1975)

1333   (20.0°C, Verschueren 1983)

1530, 1138 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.25496 – 1432.217/(210.936 + t/°C); temp range 59.74–126°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 4.7514 – 669.809/(117.657 + t/°C); temp range 24.5–94.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1529   (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.12712 – 1430.418/(210.746 + t/°C); temp range 60–126°C (Antoine eq., Dean 1985, 1992)

1664   (selected, Riddick et al. 1986)

log (P/kPa) = 6.151445 – 1368.051/(203.9298 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.176 – 1385.8/(–67.05 + T/K); temp range 332–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.13505 – 1355.816/(–70.705 + T/K); temp range: 341–399 K (Antoine eq.-II, Stephenson & Malanowski 1987)

2000, 635 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = 4.383 – 2.7134 × 10³/(T/K) + 3.9835·log (T/K) – 1.6575 × 10⁻²·(T/K) + 9.7246 × 10⁻⁶·(T/K)²; temp range 200–579 K (vapor pressure eq., Yaws 1994)

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

33.44   (exptl., Hine & Mookerjee 1975)

30.50, 31.21 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)

28.51   (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 47.6 kJ/mol, Kieckbusch & King 1979)

38.39   (predicted-MCI χ, Nirmalakhandan & Speece 1988)

82.91*   (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

20.2   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 6.400 – 2486/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.73   (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)

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

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

1.78   (24°C, shake flask-GC, Catz & Friend 1989)

1.82   (recommended, Sangster 1989, 1993)

1.78   (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, log BCF:

0.602, 1.146 (calculated-S, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.531, 2.367 (soil, calculated-S, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: using Henry's law constant, $t_{1/2}$ ~ 6.1 h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s and an estimated $t_{1/2}$ ~ 7.4 d for a 10 m deep similar model river (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

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

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

k_{OH}(calc) = 4.3×10^{-12} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 4.3×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)

photooxidation $t_{1/2}$ = 6.0 d in air was estimated for the vapor-phase reaction with an average atmospheric OH of 8×10^5/cm^3 (GEMS 1986; quoted, Howard 1990)

k_{OH} = $(41.5 \pm 3.0) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

k_{OH} = 4.2×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis: alkaline hydrolysis rate constant k = 0.087 M^{-1}·s^{-1} at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

$t_{1/2}$ = 3.1 yr, 114 d, 11.4 d at pH 7.0, 8.0, 9.0 were estimated, respectively, based on observed acid and base-catalyzed rate constants at 20°C (Mabey & Mill 1978; quoted, Howard 1990).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

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

$t_{1/2}$ = 6.0 d was estimated for the vapor-phase reaction with an average atmospheric hydroxyl radical of 8×10^5 per cm^3 (GEMS 1986; quoted, Howard 1990).

TABLE 15.1.1.8.1
Reported aqueous solubilities and Henry's law constants of butyl acetate at various temperatures

Aqueous solubility		Henry's law constant	
Stephenson & Stuart 1986		Kolb et al. 1992	
shake flask-GC/TC		equilibrium headspace-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3 mol^{-1})
0	9600	40	82.91
9.1	7600	60	203.7
19.7	6400	70	290.5
30.3	520	80	387.3
39.6	500		
50.0	500	ln (1/K_{AW}) = A −B/(T/K)	
60.2	500	A	−9.27
70.2	470	B	−3971
80.1	480		
90.5	480		
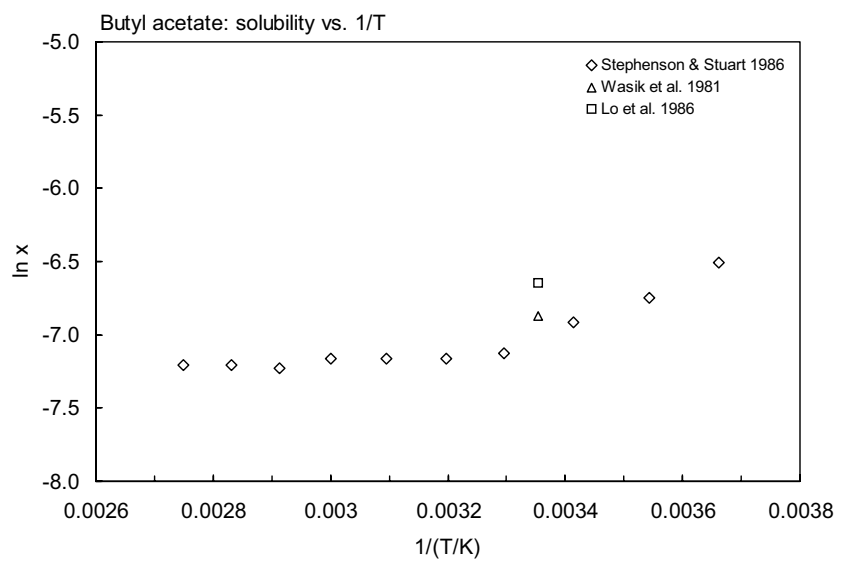
FIGURE 15.1.1.8.1 Logarithm of mole fraction solubility (In *x*) versus reciprocal temperature for butyl acetate.

TABLE 15.1.1.8.2

Reported vapor pressures of butyl acetate 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)			

Usanovich & Dembicij 1959		Kliment et al. 1964		Sheehan & Langer 1969	
in Boublik et al. 1984		**in Boublik et al. 1984**		**ebulliometry**	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.5	1560	59.74	9210	67.9	13386
33.0	2533	62.35	10426	96.3	40183
43.0	4133	65.52	11876	100	45663
51.2	6199	67.96	13159	124.0	97325
57.7	8533	71.70	15372		
65.2	11999	75.88	18252	Antoine eq.	
71.1	15332	80.49	21891	eq. 2	P/mmHg
77.5	20132	84.21	25264	A	6.9688
83.7	25598	89.58	30864	B	1326.7
88.8	31064	95.06	37543	C	199.2
94.1	42130	100.53	45356		
		107.07	56448		
eq in Boublik et al. 1984		113.62	69487		
eq. 2	P/kPa	120.62	86053		
A	4.75140	126.09	101325		
B	669.609				
C	117.657	eq in Boublik et al. 1984			
bp/°C	60.892	eq. 2	P/kPa		
	at 10 mmHg	A	6.25496		
		B	1432.217		
		C	218.936		
		bp/°C	126.116		

FIGURE 15.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for butyl acetate.
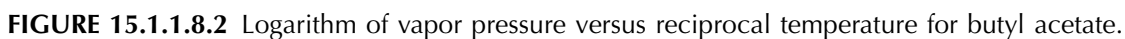
15.1.1.9 Pentyl acetate
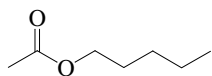
Common Name: Pentyl acetate

Synonym: acetic acid pentyl ester, amyl acetate, amylacetic ester, pentyl ethanoate, *n*-pentyl acetate, ethanoic acid pentyl ester

Chemical Name: *n*-amyl acetate, *n*-pentyl acetate

CAS Registry No: 628-63-7

Molecular Formula: $C_7H_{14}O_2$, $CH_3COOCH_2CH_2CH_2CH_2CH_3$

Molecular Weight: 130.185

Melting Point (°C):
　　–70.8　　　(Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):
　　149.2　　　(Lide 2003)

Density (g/cm³ at 20°C):
　　0.8756　　　(Weast 1982–83)
　　0.8766, 0.8719 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
　　148.5　　　(20°C, calculated-density)
　　177.4　　　(calculated-Le Bas method at normal boiling point)

Dissociation Constant:
　　24.25　　　(pK$_s$, Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
　　41.0　　　(at 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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
　　1730　　　(shake flask-turbidimeter, McBain & Richards 1946)
　　1800　　　(20°C, Verschueren 1983)
　　1700　　　(Dean 1985)
　　1700　　　(20°C, Riddick et al. 1986)
　　2200*, 1600 (19.7°C, 30.3°C, shake flask-GC/TC, measured range 0–80°C, Stephenson & Stuart 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
　　log (P/mmHg) = 8.078 – 2077/(253 + t/°C) (Davis 1946)
　　547　　　(quoted, Hine & Mookerjee 1975)
　　546　　　(quoted, Abraham 1984)
　　1290　　　(selected lit., Riddick et al. 1986)
　　log (P/kPa) = 5.4315 – 1197/(200 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
　　log (P$_L$/kPa) = 7.356 – 2258.3/(T/K); temp range 329–423 K (Antoine eq., Stephenson & Malanowski 1987)
　　log (P/mmHg) = 7.8848 – 3.0696 × 10³/(T/K) + 2.7085·log(T/K) – 1.5165 × 10^{-2}·(T/K) + 8.7135 × 10^{-6}·(T/K)²; temp range 202–598 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):
　　39.29　　　(exptl., Hine & Mookerjee 1975)
　　42.10, 42.16 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)
　　35.94　　　(vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, ΔH = 51.4 kJ/mol, Kieckbusch & King 1979)
　　48.33　　　(calculated-MCI χ, Nirmalakhandan & Speece 1988)

38.39   (calculated-molecular structure, Russell et al. 1992)
24.86   (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 7.167 - 2685/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
1.70   (calculated, Iwasa et al. 1965)
2.23   (Leo et al. 1969)
2.42   (calculated-V_I and solvatochromic parameters, Leahy 1986)

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

Bioconcentration Factor, $\log$ BCF:

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

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
　　Volatilization:
　　Photolysis:
　　Oxidation:
　　　　photooxidation $t_{1/2}$ = 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of
　　　　　　disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976).
　　Hydrolysis:
　　Biodegradation: biodegradation rates k = 0.054 d^{-1} with $t_{1/2}$ = 13 d in Lester river, k = 0.069 d^{-1} with $t_{1/2}$ = 10 d
　　　　in Superior harbor waters and k = 0.014 d^{-1} with $t_{1/2}$ = 50 d in groundwater (Vaishnav & Babeu 1987).
　　Biotransformation:
　　Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
　　Air: photooxidation $t_{1/2}$ = 2.4–24 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of
　　　　disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).
　　Surface water: biodegradation $t_{1/2}$ = 13 d in Lester river and $t_{1/2}$ = 10 d in Superior harbor waters (Vaishnav &
　　　　Babeu 1987).
　　Groundwater: biodegradation $t_{1/2}$ = 50 d (Vaishnav & Babeu 1987).
　　Sediment:
　　Soil:
　　Biota:

TABLE 15.1.1.9.1
Reported aqueous solubilities of pentyl acetate at various temperatures

Stephenson & Stuart 1986	
shake flask-GC/TC	
t/°C	S/g·m^{-3}
0	2900
19.7	2200
30.6	1600
39.5	1600
50.0	1000
60.3	1000
70.2	1700
80.1	1700
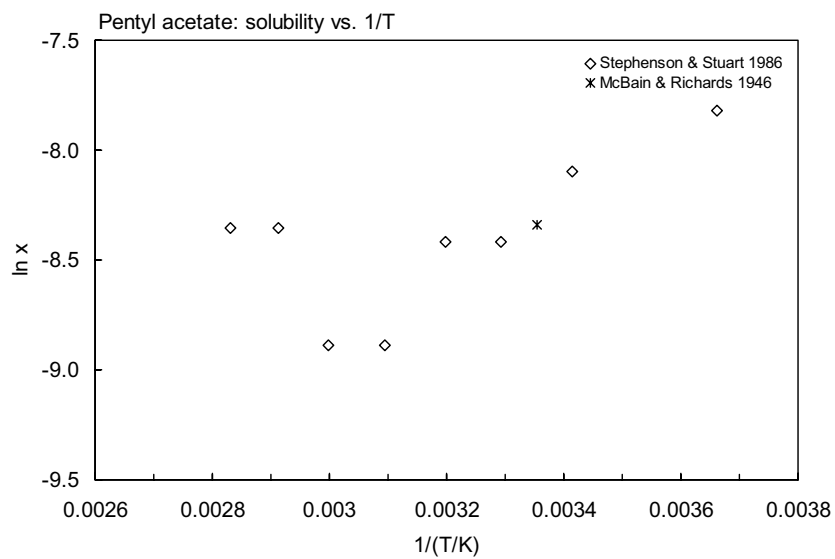
FIGURE 15.1.1.9.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for pentyl acetate.

15.1.1.10 Methyl acrylate
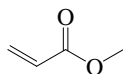
Common Name: Methyl acrylate
Synonym: acrylic acid methyl ester, methyl 2-propenoate
Chemical Name: methyl acrylate
CAS Registry No: 96-33-3
Molecular Formula: $C_4H_6O_2$, $CH_2=CHCOOCH_3$
Molecular Weight: 86.090
Melting Point (°C):
    –76.5   (Dean 1985)
Boiling Point (°C):
    80.7   (Lide 2003)
Density (g/cm³ at 20°C):
    0.9535   (Weast 1982–83; Riddick et al. 1986)
    0.9561   (Dean 1985)
Molar Volume (cm³/mol):
    90.3   (20°C, calculated-density)
    99.6   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    29.20, 33.1 (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    60000   (Dean 1985)
    49400   (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    11250   (interpolated-regression of tabulated data, temp range –43.7 to 80.2°C, Stull 1947)
    13330   (28.0°C, Stull 1947)
    log (P/mmHg) = [–0.2185 × 8598.0/(T/K)] + 8.226778; temp range –43.7 to 80.2°C (Antoine eq., Weast 1972–73)
    9330, 14660 (20°C, 30°C, Verschueren 1983)
    11000   (Riddick et al. 1986)
    3120, 5400, 9090, 11000, 14500, 30000, 70700 (0, 10, 20, 25, 30, 50, 70°C, Riddick et al. 1986)
    log (P_L/kPa) = 6.5561 – 1467.93/(–30.849 + T/K); temp range: 316–354 K (Antoine eq., Stephenson & Malanowski 1987)
    log (P/mmHg) = 47.0416 – 3.1218 × 10³/(T/K) – 14.86·log(T/K) + 7.1646 × 10⁻³·(T/K) + 3.4547 × 10⁻⁶·(T/K)²; temp range 196–536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):
    19.17   (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW}:
    0.21   (Tute 1971; Laurence et al. 1972)
    0.36   (HPLC-RT correlation, Fujisawa & Masuhara 1981)
    0.80   (shake flask-GC, Tanii & Hashimoto 1982)
    0.80   (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, or Half-Lives, $t_{1/2}$:

    Volatilization:

    Photolysis:

    Oxidation: photooxidation $t_{1/2}$ = 2.7–27 h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991)

    Hydrolysis: first order hydrolysis $t_{1/2}$ = 2.8 yr at pH 7 and 25°C, based on measured base rate constant; acid rate constant k = 1.2×10^{-7} $M^{-1} \cdot h^{-1}$ using measured rate constant for ethyl acrylate, resulting a $t_{1/2}$ = 280 yr; base rate constant k = 0.0779 $M^{-1} \cdot h^{-1}$ at pH 9 and 25°C with $t_{1/2}$ = 10 d (Roy 1972; quoted, Howard et al. 1991).

    Biodegradation: aqueous aerobic $t_{1/2}$ = 24–168 h, based on biological screening test data (Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 96–672 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

    Biotransformation:

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

Half-Lives in the Environment:

    Air: photooxidation $t_{1/2}$ = 2.7–27 h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991);

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

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

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

    Sediment:

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

    Biota:

15.1.1.11 Ethyl acrylate
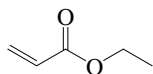
Common Name: Ethyl acrylate
Synonym: acrylic acid ethyl ester, ethyl 2-propenoate, propenoic acid ethyl ester
Chemical Name: ethyl acrylate, *n*-ethyl acrylate
CAS Registry No: 140-88-5
Molecular Formula: $C_5H_8O_2$, CH_2=CHCOOCH$_2$CH$_3$
Molecular Weight: 100.117
Melting Point (°C):
   –71.2   (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
   99.4   (Lide 2003)
Density (g/cm³ at 20°C):
   0.9234   (Weast 1982–83; Riddick et al. 1986)
   0.9405   (Dean 1985)
Molar Volume (cm³/mol):
   109.2   (Stephenson & Malanowski 1987)
   123.8   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   34.7   (at 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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   20000   (Verschueren 1983)
   15000   (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
   designated * are compiled at the end of this section):
   4860*   (interpolated-regression of tabulated data, temp range –29.5 to 99.5°C, Stull 1947)
   log (P/mmHg) = [–0.2185 × 9259.4/(T/K)] + 8.347017; temp range –29.5 to 99.5°C (Antoine eq., Weast 1972–73)
   3866, 6532 (20°C, 30°C, Verschueren 1983)
   5100   (lit average, Riddick et al. 1986)
   log (P/kPa) = 7.2103 – 1939.49/(T/K), temp range: not specified, (Antoine eq., Riddick et al. 1986)
   5140   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
   log (P_L/kPa) = 6.25041 – 1354.65/(–53.603 + T/K); temp range: 244–373 K (Antoine eq., Stephenson &
      Malanowski 1987)
   log (P/mmHg) = 55.0109 – 3.5904 × 10³/(T/K) – 17.694·log(T/K) + 8.051 × 10⁻³·(T/K) – 4.8864 × 10⁻¹³·(T/K)²;
      temp range 202–553 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol 25°C):
   34.041   (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW}:
   0.73   (Tute 1971; Laurence et al. 1972)
   0.88   (calculated-fragment const. per Rekker 1977, Hermens & Leeuwangh 1982)
   0.66   (HPLC-RT correlation, Fujisawa & Masuhara 1981)
   1.33   (shake flask-GC, Tanii & Hashimoto 1982)
   1.32   (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, or Half-Lives, $t_{1/2}$:
  Volatilization:
  Photolysis:
  Oxidation: photooxidation $t_{1/2}$ = 2.37–22.7 h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
  Hydrolysis: overall rate constant k_h = 6.3×10^{-9} s^{-1} with $t_{1/2}$ = 3.5 yr at 25°C and pH 7; acid rate constant k_A = 1.2×10^{-13} s^{-1} and base rate constant k_B = 7.8×10^{-9} s^{-1} at 25° and pH 7 (Mabey & Mill 1978)
    $t_{1/2}$ = 2.8 yr at pH 7 and 25°C, based on acid and base catalyzed hydrolysis rate constants; acid rate constant k_A = 1.2×10^{-6} M^{-1} s^{-1} with $t_{1/2}$ = 244 yr at pH 5; measured base rate constant k_B = 0.078 $M^{-1} \cdot h^{-1}$ with $t_{1/2}$ = 10.4 d at pH 9 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991);
    calculated rate constant for base-catalyzed hydrolysis k_B = 5.0×10^{-2} M^{-1} s^{-1} and estimated $t_{1/2}$ ~ 25 d in aqueous solutions at pH 8.8 (Freidig et al. 1999).
  Biodegradation: aqueous aerobic $t_{1/2}$ = 24–168 h, based on aqueous aerobic screening test data (Price et al. 1974; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
  Air: photooxidation $t_{1/2}$ = 2.37–22.7 h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).
  Surface water: hydrolysis $t_{1/2}$ = 3.5 yr at 25°C and pH 7 (Mabey & Mill 1978)
    $t_{1/2}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  Groundwater: $t_{1/2}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  Sediment:
  Soil: $t_{1/2}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  Biota:

TABLE 15.1.1.11.1
Reported vapor pressures of ethyl acrylate at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
–29.5	133.3
–8.70	666.6
2.0	1333
13.0	2666
26.0	5333
33.5	7999
44.5	13332
61.5	26664
80.0	53329
99.5	101325
mp/°C	–71.2
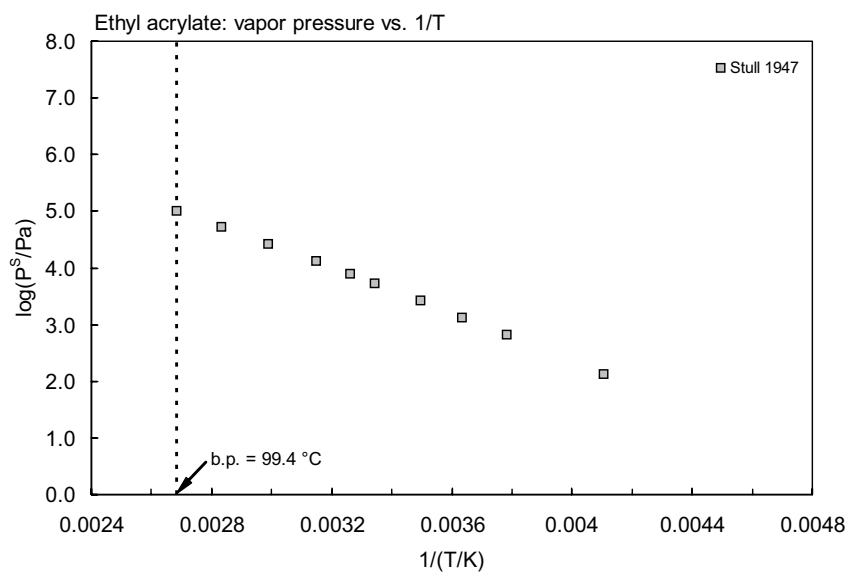
FIGURE 15.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl acrylate.

15.1.1.12 Methyl methacrylate
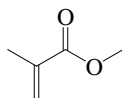
Common Name: Methyl methacrylate
Synonym: methyl 2-methyl-2-propenoate, methyl ester methacrylic acid, methacrylic acid methyl ester, MMA
Chemical Name: 2-methyl-2-propenoic acid methyl ester
CAS Registry No: 80-62-6
Molecular Formula: $C_5H_8O_2$, $H_2C=C(CH_3)COOCH_3$
Molecular Weight: 100.117
Melting Point (°C):
   –47.55   (Lide 2003)
Boiling Point (°C):
   100.5   (Lide 2003)
Flash Point (°C): 10
Density (g/cm³ at 20°C):
   0.9440   (Weast 1982–83)
Molar Volume (cm³/mol):
   106.6   (25°C, Stephenson & Malanowski 1987)
   121.8   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
   40.7, 36.0   (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
   16000   (Dean 1985)
   15000   (USEPA 1985; ENVIROFATE; ISHOW)
   15900   (Yalkowsky et al. 1987)
   15600   (20°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures
   designated * are compiled at the end of this section):
   5332*, 4888 (25.5°C, interpolated-regression of tabulated data, temp range –30.5 to 101°C, Stull 1947)
   1315*   (3.44°C, temp range –45.26 to 3.44°C, Bywater 1952; quoted, Boublik et al. 1984)
   log (P/mmHg) = [–0.2185 × 8794.9/(T/K)] + 8.140942; temp range –30.5 to 101°C (Antoine eq., Weast 1972–73)
   3732, 5333   (20°C, 26°C, Verschueren 1977, 1983)
   7003*   (32.489°C, temp range 32.489–99.855°C, Boublik & Aim 1979; quoted, Boublik et al. 1984)
   5333   (25.5°C, Weast 1982–83)
   4440   (extrapolated average-Antoine eq., Boublik et al. 1984)
   log (P/kPa) = 3.20496 – 4017.882/(126.685 + t/°C); temp range –45.26 to 3.44°C (Antoine eq. from reported
       exptl. data, Boublik et al. 1984)
   log (P/kPa) = 6.19400 – 1315.670/(213.490 + t/°C); temp range: 32.41–99.855°C (Antoine eq. from reported
       exptl. data, Boublik et al. 1984)
   4846   (extrapolated-Antoine equation, Dean 1985)
   log (P/mmHg) = 8.4092 – 2050.5/(274.4 + t/°C); temp range: 39–89°C (Antoine eq., Dean 1985, 1992)
   5100   (lit. average, Riddick et al. 1986)
   log (P/kPa) = 7.83859 – 2126.21/(T/K), temp range 0–30°C (Antoine eq., Riddick et al. 1986)
   5081, 5020   (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
   log (P_L/kPa) = 6.63751 – 1597.9/(–28.76 + T/K); temp range: 293–374 K (Antoine eq.-I, Stephenson &
       Malanowski 1987)

log $(P_L/kPa) = 6.43088 – 1461.197/(–43.15 + T/K)$; temp range: 293–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/mmHg) = 106.896 – 5.2741 \times 10^3/(T/K) – 37.654 \cdot log(T/K) + 1.862 \times 10^{-2} \cdot (T/K) – 3.6507 \times 10^{-13} \cdot (T/K)^2$; temp range 225–564 K (vapor pressure eq., Yaws 1994)

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

24.31	(calculated-P/C, USEPA 1985)
32.823	(calculated-P/C, Howard 1989)
32.09	(calculated-P/C, this work)

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

0.73	(Tute 1971; Laurence et al. 1972)
0.70	(shake flask, Fujisawa & Masuhara 1981)
0.67	(HPLC-RT correlation, Fujisawa & Masuhara 1981)
1.36	(CLOGP, Hansch & Leo 1982)
1.38	(shake flask-GC, Tanii & Hashimoto 1982)
0.79	(calculated-f const. as per Lyman et al. 1982, USEPA 1985)
1.38	(recommended, Sangster 1989)
1.38	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

–0.03	(correlated as per Veith et al. 1979 for aquatic organisms, USEPA 1985)
0.55	(calculated-K_{OW}, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

1.80	(calculated-K_{OW} as per Lyman et al. 1982, USEPA 1985)
1.94	(calculated-K_{OW}, Howard 1989)
0.74	(calculated-K_{OW}, Kollig 1993)

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

Volatilization: $t_{1/2} = 6.3$ h from model river water (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: photodegradation $t_{1/2} = 2.7$ h in air of urban areas and $t_{1/2} > 3$ h in rural areas (Joshi et al. 1982; quoted, Howard 1989) (CHEMFATE; Hazardous Substance Databank).

Oxidation: photooxidation $t_{1/2} = 1.1–9.7$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: alkaline hydrolysis rate constant at 25°C, $k = 171$ M^{-1} h^{-1} (Sharma & Sharma 1970; quoted, Ellington et al. 1987; Ellington 1989);

alkaline catalyzed rate constant k(exptl) = 200 M^{-1}·h^{-1} at 25°C with estimated $t_{1/2} \sim 3.9$ yr at pH 7 and $t_{1/2} = 14$ d at pH 9 (Ellington et al. 1987; quoted, Ellington 1989; Howard 1989; Howard et al. 1991; Kollig 1993);

hydrolysis $t_{1/2} = 4$ yr at pH 7 and 25°C; base rate constant k = 200 M^{-1} h^{-1} with $t_{1/2} = 14.4$ d at pH 9 based on measured rate constant at 25°C and pH 11 (Howard et al. 1991)

k(calc) = 9.0×10^{-7} M^{-1} s^{-1}, 2.6×10^{-2} M^{-1} s^{-1} for neutral and base-catalyzed hydrolysis and estimated $t_{1/2} \sim 8$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999)

Biodegradation: completely degraded by activated sludge in approximately 20 h (Slave et al. 1974; quoted, EPA 1985; Howard 1989; Hazardous Substance Databank);

expert systems survey found that both aerobic ultimate degradation in receiving waters and anaerobic ultimate degradation were within a month and aerobic primary degradation in receiving waters was within few days (Boethling et al. 1989);

aqueous aerobic $t_{1/2} = 168–672$ h, based on unacclimated screening test data (Pahren & Bloodgood 1961; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672–2688$ h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 1.1–9.7 h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 to 1–5 d (Kelly et al. 1994).

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

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

Sediment:

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

Biota:

TABLE 15.1.1.12.1
Reported vapor pressures of methyl methacrylate 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		Bywater 1952		Boublik & Aim 1979	
summary of literature data		in Boublik et al. 1984		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–30.5	133.3	–45.26	17	32.489	7003
–10.0	666.6	–43.46	25	37.962	9160
1.0	1333	–40.16	43	38.307	9306
11.0	2666	–35.16	64	43.731	12004
25.5	5333	–32.06	95	43.834	12049
34.5	7999	–27.96	140	47.951	14515
47.0	13332	–22.96	223	48.225	14680
63.0	26664	–20.46	260	53.954	18815
82.0	53329	–16.76	347	53.289	18290
101.0	101325	–10.56	547	55.846	20379
		–3.46	893	61.670	25849
mp/°C	-	–0.16	1053	65.350	29910
		3.44	1315	69.772	35421
				74.142	41676
		in Boublik et al. 1984		79.113	49831
		eq. 2	P/kPa	84.938	61430
		A	3.20496	91.998	77126
		B	401.882	99.855	98890
		C	126.685		
		bp/°C	–1.292	in Boublik et al. 1984	
			at 1 mmHg	eq. 2	P/kPa
				A	6.19400
				B	1315.670
				C	215.490
				bp/°C	100.641
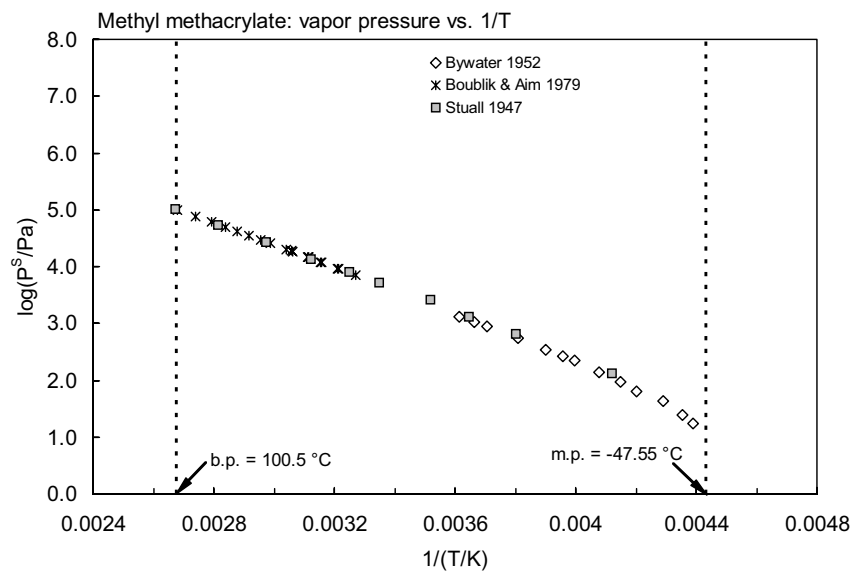
FIGURE 15.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for methyl methacrylate.

15.1.2 Aromatic esters

15.1.2.1 Methyl benzoate
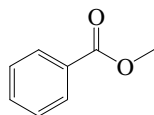
Common Name: Methyl benzoate
Synonym: benzoic acid methyl ester
Chemical Name: methyl benzoate
CAS Registry No: 93-58-3
Molecular Formula: $C_8H_8O_2$, $C_6H_5COOCH_3$
Molecular Weight: 136.149
Melting Point (°C):
    –12.4   (Lide 2003)
Boiling Point (°C):
    199   (Lide 2003)
Density (g/cm³ at 20°C):
    1.08854, 1.08377   (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
    125.0   (Stephenson & Malanowski 1987)
    151.2   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    41.18, 55.84   (normal bp, 25°C, Dreisbach 1955)
    43.18, 55.568   (normal bp, 25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.736   (Dreisbach 1955; Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
    1524   (titration, Booth & Everson 1948)
    4018   (Hine & Mookerjee 1975)
    2100   (20°C, quoted, Riddick et al. 1986)
    1600   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
    2130*, 2820 (20.1°C, 29.6°C, shake flask-GC/TC, measured range 0–90.5°C, Stephenson & Stuart 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    log (P/mmHg) = 7.48253 – 1974.6/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
    52.58   (calculated by formula, Dreisbach 1955)
    log (P/mmHg) = 7.07832 – 1656.25/(195.23 + t/°C); temp range: 100–260°C (Antoine eq. for liquid state, Dreisbach 1955)
    log (P/mmHg) = [–0.2185 × 12077.2/(T/K)] + 8.509910; temp range: 39–199.5°C (Antoine eq., Weast 1972–73)
    77.6   (extrapolated-Antoine eq., Dean 1985)
    log (P/mmHg) = 6.60743 – 1974.6/(230.0 + t/°C); temp range 111–199°C (Antoine eq., Dean 1985, 1992)
    52.58   (quoted lit. average, Riddick et al. 1986)
    log (P/kPa) = 6.60743 – 1974.6/(230 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
    54.5   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 8.183 – 2816.6/(T/K); temp range 283–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.20322 – 1656.25/(–77.92 + T/K); temp range: 383–533 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log $(P/mmHg)$ = –13.6342 –2.9133 × 10^3/(T/K) + 11.773·log (T/K)–2.3979 × 10^{-2}·(T/K) + 1.1324 × 10^{-5}·(T/K)^2; temp range 261–693 K (vapor pressure eq., Yaws 1994)

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

1.80   (calculated-C_W/C_A, Hine & Mookerjee 1975)
2.48   (calculated-bond contribution, Hine & Mookerjee 1975)

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

2.15   (HPLC-RT correlation, D'Amboise & Hanai 1982)
2.22   (HPLC-k′ correlation, Haky & Young 1984)
2.14   (shake flask-HPLC, Nielson & Bundgaard 1988)
2.10   (recommended, Klein et al. 1988)
2.15   (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.20   (recommended, Sangster 1989)
2.12   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.30, 2.01, 1.98   (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
1.89   (calculated-MCI χ, Meylan et al. 1992)
2.10   (quoted or calculated-QSAR MCI ^{1}χ, Sabljic et al. 1995)
2.14; 2.57, 2.14, 1.94, 2.16, 1.89   (soil: calculated-K_{OW}; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: overall rate constant k_h = 1.90 × 10^{-10} s^{-1} with t$_{1/2}$ = 118 yr at 25°C and pH 7 (Mabey & Mill 1978)
          alkaline hydrolysis rate constant k = 0.0794 M^{-1} s^{-1} (Drossman et al. 1988, quoted, Collette 1990)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants::

Half-Lives in the Environment:

Air:
Surface water: hydrolysis t$_{1/2}$ = 118 yr at 25°C and pH 7 (Mabey & Mill 1978)
Groundwater:
Sediment:
Soil:
Biota:

TABLE 15.1.2.1.1
Reported aqueous solubilities of methyl benzoate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	S/g·m^{-3}
0	2210
9.7	2210
20.1	2130
29.6	2820
40.2	2470
49.8	2580
60.1	2860
70.2	3250
80.3	3580
90.5	4080
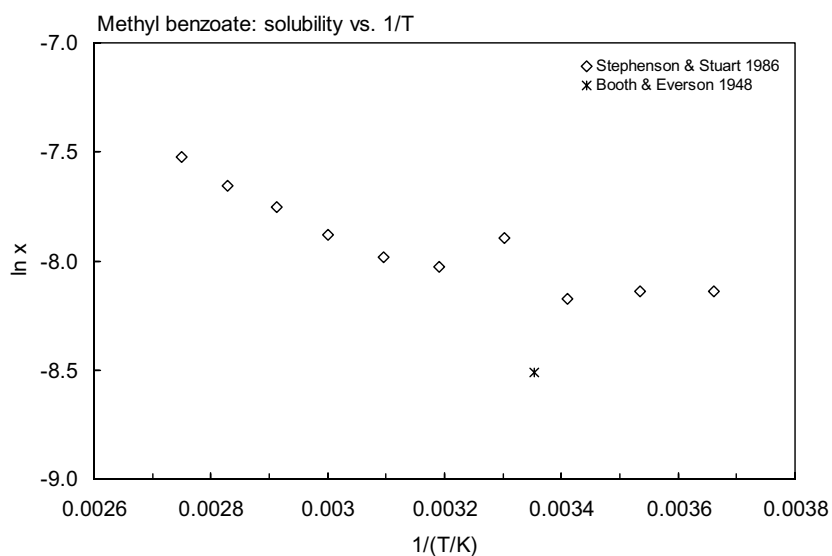
FIGURE 15.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for methyl benzoate.

15.1.2.2   Ethyl benzoate
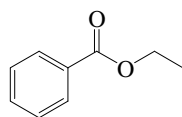
Common Name: Ethyl benzoate
Synonym: benzoic acid ethyl ester, ethyl benzenecarboxylate
Chemical Name: benzoic acid ethyl ester, ethyl benzenecarboxylate, ethyl benzoate
CAS Registry No: 93-89-0
Molecular Formula: $C_9H_{10}O_2$, $C_6H_5COOC_2H_5$
Molecular Weight: 150.174
Melting Point (°C):
      –34   (Lide 2003)
Boiling Point (°C):
      212   (Lide 2003)
Density (g/cm³ at 20°C):
      1.0468   (Weast 1982–83)
      1.0511, 1.0372 (15°C, 30°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
      175.0   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
      40.5   (Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
      compiled at the end of this section):
      720   (Seidell 1941; quoted, Andrews & Keefer 1950)
      598   (Deno & Berkheimer 1960)
      702   (calculated-K_{OW}, Hansch et al. 1968)
      510   (calculated-K_{OW}, Yalkowsky & Morozowich 1980)
      2026   (calculated-K_{OW} and mp, Amidon & Williams 1982),
      807   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)
      1090   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Kamlet et al. 1987)
      464   (calculated-intrinsic molar volume V_I and mp, Kamlet et al. 1987)
      500   (20°C, Riddick et al. 1986)
      926   (calculated-fragment const., Wakita et al. 1986)
      398   (calculated-MCI χ, Nirmalakhandan & Speece 1988)
      850*, 810   (19.6°C, 30. °C, shake flask-GC/TC, measured range 0–90.3°C, Stephenson & Stuart 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
      42.1   (extrapolated-regression of tabulated data, temp range 44–213.4°C, Stull 1947)
      $\log (P/mmHg) = [–0.2185 \times 11981.5/(T/K)] + 8.279591$; temp range 44–213.4°C (Antoine eq., Weast 1972–73)
      24.0   (20°C, quoted lit., Riddick et al. 1986)
      $\log (P/kPa) = 7.7579 – 2750.0/(T/K)$; temp range 90–140°C (Antoine eq., Riddick et al. 1986)
      $\log (P/kPa) = 7.1599 – 2500.0/(T/K)$; temp range 140–220°C (Antoine eq., Riddick et al. 1986)
      27.5   (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
      $\log (P_L/kPa) = 6.81152 – 2174.3/(–34.071 + T/K)$; temp range 358–487 K (Antoine eq.-I, Stephenson & Malanowski
         1987)
      $\log (P_L/kPa) = 8.23958 – 2922.167/(T/K)$; temp range 288–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 40.8047 - 3.9985 \times 10^3/(T/K) - 11.793 \cdot \log (T/K) + 4.0697 \times 10^{-3} \cdot (T/K) - 1.2372 \times 10^{-13} \cdot (T/K)^2$; temp range 238–698 K (vapor pressure eq., Yaws 1994)

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

  10.298   (calculated-P/C with selected values)

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

  2.62   (calculated, Hansch et al. 1968)
  2.20   (shake flask-spectrophotometry, Yaguzhinskii et al. 1973)
  2.64   (Valvani et al. 1981, Amidon & Williams 1982)
  2.64   (shake flask-HPLC, Nielsen & Bundgaard 1988)
  2.60   (recommended, Klein et al. 1988)
  2.64   (recommended, Sangster 1989)
  2.66, 2.89, 2.90   (centrifugal partition chromatography CPC-RV, Gluck & Martin 1990)
  2.70 ± 0.15, 2.63 ± 0.57 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
  2.64   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

  2.25, 2.17, 2.43   (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
  2.16   (calculated-MCI χ and fragment contribution, Meylan et al. 1992)
  2.30   (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

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

  Volatilization:
  Photolysis:
  Oxidation:
  Hydrolysis: overall rate constant $k_h = 3.0 \times 10^{-9}$ s^{-1} with $t_{1/2} = 7.3$ yr at 25°C and pH 7 (Mabey & Mill 1978)
      alkaline hydrolysis rate constant $k = 0.0316$ M^{-1} s^{-1} (Drossman et al. 1988, quoted, Collette 1990)
  Biodegradation:
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

  Air:
  Surface water: hydrolysis $t_{1/2} = 7.3$ yr at 25°C and pH 7 (Mabey & Mill 1978)
  Groundwater:
  Sediment:
  Soil:
  Biota:

TABLE 15.1.2.2.1
Reported aqueous solubilities of ethyl benzoate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	S/g·m⁻³
0	1080
19.6	850
30.5	810
40.0	1060
50.0	1080
60.1	1170
70.5	1210
80.2	1210
90.3	1430
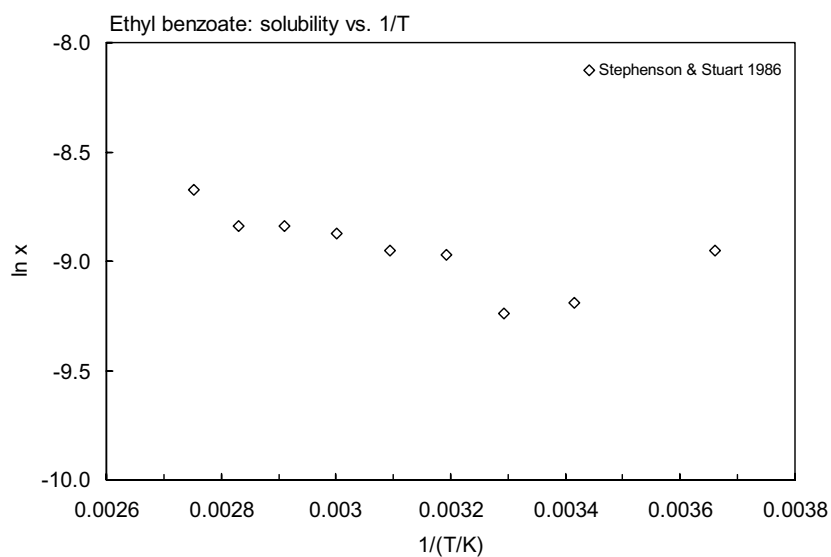
FIGURE 15.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl benzoate.

15.1.2.3 *n*-Propyl benzoate
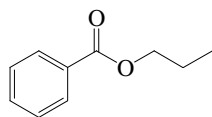
Common Name: *n*-Propyl benzoate
Synonym: benzoic acid *n*-propyl ester, propyl benzenecarboxylate
Chemical Name: benzoic acid *n*-propyl ester, propyl benzenecarboxylate, propyl benzoate
CAS Registry No: 2315-68-6
Molecular Formula: $C_{10}H_{12}O_2$, $C_6H_5COOCH_2CH_2CH_3$
Molecular Weight: 164.201
Melting Point (°C):
    –51.6   (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
    211   (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
    1.0232   (Riddick et al. 1986)
Molar Volume (cm³/mol):
    160.5   (20°C, calculated-density, Stephenson & Malanowski 1987)
    199.4   (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    51.92; 49.75 (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 (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    350   (quoted exptl., Kamlet et al. 1987)
    292   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Kamlet et al. 1987)
    140   (calculated-intrinsic molar volume V_I and mp, Kamlet et al. 1987)
    966   (calculated-MCI χ, Nirmalakhandan & Speece 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
    133.3   (54.6°C, summary of literature data, temp range 54.6–231°C, Stull 1947)
    $\log (P/mmHg) = [-0.2185 \times 12318.7/(T/K)] + 8.237827$; temp range 54.6–231°C (Antoine eq., Weast 1972–73)
    100   (54.6°C, Riddick et al. 1986)
    $\log (P/kPa) = 7.42756 - 2172.71/(T/K)$; temp range 80–160°C (Antoine eq., Riddick et al. 1986)
    $\log (P_L/kPa) = 6.68614 - 2165.28/(-41.593 + T/K)$; temp range 327–504 K (Antoine eq., Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, $\log K_{OW}$:
    1.80   (shake flask-HPLC, Nielsen & Bundgaard 1988)
    3.18   (recommended, Sangster 1989)
    3.01   (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

15.1.2.4   Benzyl benzoate
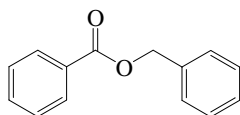
Common Name: Benzyl benzoate

Synonym: benzoic acid benzyl ester, phenylmethyl benzoate, benzyl benzenecarboxylate, benzyl phenylformate, benzenoate

Chemical Name: benzyl benzoate, phenylmethyl benzoate, benzyl benzenecarboxylate

CAS Registry No: 120-51-4

Molecular Formula: $C_{14}H_{12}O_2$, $C_6H_5COOCH_2C_6H_5$

Molecular Weight: 212.244

Melting Point (°C):
    19.4   (Riddick et al. 1986)

Boiling Point (°C):
    323.5   (Lide 2003)

Density (g/cm³ at 20°C):
    1.1121   (25°C, Weast 1982–83)
    1.120, 1.1121 (19.5°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
    190.9   (25°C, calculated-density)
    243.6   (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):
    53.56   (at normal bp, Hon et al. 1976)
    77.8; 53.6   (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 (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    15.73   (Seidell 1941; quoted, Deno & Berkheimer 1960)
    61.21   (calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

    log (P/mmHg) 6.42726 – 1594.49/(126.36 + t/°C); temp range 224.7–329.09°C (Antoine eq., from twin ebulliometry measurement, Hon et al. 1976)
    0.0137   (extrapolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 5.59354 – 1628.726/(130.735 + t/°C); temp range 224.7–329°C (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)
    461   (150°C, quoted lit., Riddick et al. 1986)
    0.0104   (calculated-Antoine eq., 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)
    0.043   (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 9.240 – 4057/(T/K); temp range 297–353 K (Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P_L/kPa) = 5.63847 – 1666.706/(–137.564 + T/K); temp range 497–602 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = –1.654 – 4.6284 × 10³/(T/K) + 7.363·log (T/K) – 1.8259 × 10⁻²·(T/K) + 7.4580 × 10⁻⁶·(T/K)²; temp range 293–820 K (vapor pressure eq., Yaws et al. 1994)
    0.0178, 0.0107, 0.0135, 0.295, 0.0603   (GC-RT correlation, Sugden's parachor method, McGowan's parachor method, calculated-MCI, calculated-MW, Tsuzuki 2001)

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

    0.57   (calculated-P/C with selected values)

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

    3.86   (quoted, calculated-V_I and solvatochromic parameters, Taft et al. 1985)
    4.00   (quoted, calculated-V_I and solvatochromic parameters, Leahy 1986)
   3.97   (recommended value, Sangster 1989)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:
    Photolysis:
    Hydrolysis:
    Oxidation:
    Hydrolysis: overall rate constant $k_h = 8.0 \times 10^{-10}$ s^{-1} with $t_{1/2}$ = 27 yr at 25°C and pH 7 (Mabey & Mill 1978)
        alkaline hydrolysis rate constant k = 0.00794 M^{-1} s^{-1} (Mabey et al. 1978; quoted, Collette 1990)
    Biodegradation:
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

    Air:
    Surface water: hydrolysis $t_{1/2}$ = 27 yr at 25°C and pH 7 (Mabey & Mill 1978)
    Groundwater:
    Sediment:
    Soil:
    Biota:

15.1.3 PHTHALATE ESTERS

15.1.3.1 Dimethyl phthalate (DMP)
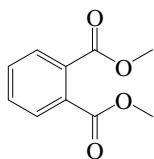
Common Name: Dimethyl phthalate
Synonym: DMP, 1,2-benzenedicarboxylic acid dimethyl ester, dimethyl-1,2-benzenedicarboxylate, methyl Common phthalate, o-dimethylphthalate, phthalic acid dimethyl ester
Chemical Name: dimethyl phthalate, dimethyl-o-phthalate, methyl phthalate
CAS Registry No: 131-11-3
Molecular Formula: $C_{10}H_{10}O_4$, o-$C_6H_4(COOCH_3)_2$
Molecular Weight: 194.184
Melting Point (°C):
    5.5   (Lide 2003)
Boiling Point (°C):
    283.7   (Lide 2003)
Density (g/cm³ at 20°C):
    1.189   (25°C, Fishbein & Albro 1972)
    1.1905   (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
    162.8   (calculated-density, Stephenson & Malanowski 1987)
    206.4   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    78.66   (Small et al. 1948)
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):
    3965   (Deno & Berkheimer 1960)
    5000   (20°C, Fishbein & Albro 1972)
    4000   (32°C, from Monsanto Chemical Co. data sheets, Peakall 1975)
    4320 ± 37 (shake flask-GC, Wolfe et al. 1980b; Wolfe et al. 1980a)
    4248   (shake flask-LSC, Veith et al. 1980)
    4290   (20°C, shake flask-UV, Leyder & Boulanger 1983)
    5000, 1744 (20°C, Verschueren 1983)
    4000 ± 60 (shake flask-HPLC/UV, Howard et al. 1985)
    2810   (21°C, shake flask-HPLC/UV, Nielsen & Bundgaard 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):
    40*   (82°C, ebulliometry, measured range 82–151°C, Gardner & Brewer 1937)
    log (P/mmHg) = 9.117 –1496.375/(T/K); temp range 82–151°C (Antoine eq. derived by Kim 1985 from exptl data of Gardner & Brewer 1937)
    0.863*   (extrapolated-regression of tabulated data, temp range 100.3–288.7°C Stull 1947)
    0.245   (effusion method, extrapolated-Antoine eq., Small et al. 1948)
    log (P/mmHg) = 11.06 – 4113/(T/K); temp range 32–55°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)
    0.559   (20°C, calculated-Antoine eq., Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 14922.2/(T/K)] + 8.747053; temp range 100.3–287°C (Antoine eq., Weast 1972–73)
    0.445   (gas saturation, extrapolated, measured range 60–100°C, Potin-Gautier et al. 1982)

log (P/mmHg) = 8.899 – 3332.764/(T/K); temp range 60–100°C (Antoine eq., Potin-Gautier et al. 1982)

log (P/kPa) = 3.64598 – 699.876/(51.372 + t/°C); temp range 82–151°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 4.52232 – 700.31/(51.42 + t/°C); temp range 82–151°C (Antoine eq., Dean 1985, 1992)

0.220   (gas saturation-HPLC/UV, Howard et al. 1985; quoted, Howard et al. 1986; Howard 1989; Banerjee et al. 1990)

0.245, 0.863   (extrapolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 10.185 – 4113/(T/K); temp range 304–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.095 – 3327/(T/K); temp range 371–547 K (Antoine eq.-II, Stephenson & Malanowski 1987)

1.190   (GC-RT correlation, Hinckley et al. 1990)

log (P/mmHg) = 12.6974 – 4.1989 × 10^3/(T/K) + 0.3463·log(T/K) – 7.6524 × 10^{-3}·(T/K) + 3.349 × 10^{-6}·(T/K)^2; temp range 272–766 K (vapor pressure eq., Yaws et al. 1994)

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

0.111   (calculated-P/C, Fishbein & Albro 1972)

0.111   (calculated-P/C, Wolfe et al. 1980a)

0.011   (calculated as per Lyman et al. 1982; quoted, Howard 1989)

0.218   (20°C, calculated-P/C, Mabey et al. 1982)

0.012   (selected, Staples et al. 1997)

0.00978   (calculated-QSPR, Cousins & Mackay 2000)

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

1.61   (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1983)

1.56   (HPLC-RT correlation, Veith et al. 1980)

1.62, 1.82   (HPLC-k′ correlations, McDuffie 1981)

1.53   (20°C, shake flask-UV, Leyder & Boulanger 1983)

1.47, 1.90   (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)

1.56   (shake flask, unpublished data, Hansch & Leo 1985; 1987)

1.66   (shake flask, average from interlaboratory study, Renberg et al. 1985)

1.74, 1.61   (HPLC, RP-TLC, average from interlaboratory study, Renberg et al. 1985)

1.62   (HPLC-RT correlation, Eadsforth 1986)

1.46   (shake flask-HPLC/UV, Nielsen & Bundgaard 1989)

1.56   (recommended, Sangster 1993)

1.56   (recommended, Hansch et al. 1995)

1.61   (recommended, Staples et al. 1997)

1.54   (micro-emulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

7.01   (calculated-QSPR, Cousin & Mackay 2000)

Bioconcentration Factor, log BCF:

0.67   (calculated-K_{OW}, Veith et al. 1979, 1980)

1.76   (bluegill sunfish, Barrows et al. 1980)

1.76   (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1983)

1.42   (bacteria, calculated-K_{OW}, Wolfe et al. 1980a)

0.49–0.8, 0.67–0.78   (shrimp, fish, Wofford et al. 1981)

1.20   (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

0.77   (sheepshead minnow, quoted from Wofford et al. 1981, Zaroogian et al. 1985)

1.76, 2.22   (quoted, calculated-MCI χ, Sabljic 1987)

0.67, 0.73   (brown shrimp, sheepshead minnow, quoted, Howard 1989)

1.76   (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

1.64   (soil, estimated, Kenaga 1980)

2.20   (soil, estimated-K_{OW}, Wolfe et al. 1980a)

1.74   (soil/sediment, Osipoff et al. 1981)
1.24   (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.52   (sediment, calculated-K_{OW}, Pavlou & Weston 1983, 1984)
2.69   (activated carbon, calculated- MCI χ, Blum et al. 1994)
1.20   (calculated-K_{OW}, Kollig 1993)
1.60   (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
4.70   (suspended solids, calculated-K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)
1.64, 2.14; 2.16, 1.87, 2.53, 1.83, 1.67 (soil: quoted lit., calculated-K_{OW}; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization: estimated $t_{1/2} = 46$ d from a river of 1 m deep with 1.0 m/s current and a 3.0 m/s wind using calculated Henry's law constant and considering the volatilization rate being controlled by the diffusion through the air layer (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: direct $k_P = 2 \times 10^{-4}$ h^{-1} (EXAMS model, Wolfe et al. 1980a);
     abiotic degradation $t_{1/2} = 3500$ h for direct sunlight in surface waters and $t_{1/2} = 12.7$ h in pure water but reduced to 2.8 h in the presence of NO_2 when irradiated with a UV lamp through a Pyrex filter (Howard 1989)
     Indirect photolysis rate $k = 0.048$ d^{-1} with $t_{1/2} = 14.4$ d in air (Peterson & Staples 2003)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
     k(aq.) = 18 M^{-1} s^{-1} for reaction with free radical in aqueous environment (Wolfe et al. 1980a)
     k(aq.) << 360 M^{-1} h^{-1} for singlet oxygen and 0.05 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)
     photooxidation $t_{1/2} = 23.8$ h (estimated, Howard 1989)
     atmospheric $t_{1/2} = 112–1118$ h, based on estimated rate data for the reaction with OH radical in air (Howard et al. 1991)
     k(aq.) = (0.20 ± 0.10) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21 ± 1°C, with a $t_{1/2} = 1.9$ d at pH 7 (Yao & Haag 1991).
     k(aq.) = 4 × 10^9 M^{-1} s^{-1} for the reaction with OH radical in aqueous solution (Haag & Yao 1992)
     photooxidation $t_{1/2}$(predicted) = 9.3–93 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)
     $k_{OH} = 5.74 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} and $t_{1/2} = 14.4$ d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis: k(acid-catalyzed) = 0.04 M^{-1} h^{-1}, k(alkaline) = 2.5 × 10^2 M^{-1} h^{-1}; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ month to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)
     k(second-order alkaline) = 6.9 × 10^{-2} M^{-1} s^{-1} at pH 8 and 30°C, and $t_{1/2} = 4$ months for hydrolytic degradation in the eutrophic lake system (Wolfe et al. 1980b; quoted, Kollig 1993)
     k(second-order alkaline) = 6.9 × 10^{-2} M^{-1} s^{-1} at pH 10–12 and 30°C in water with $t_{1/2}$(calc) = 3.2 yr at pH 7 (Callahan et al. 1979)
     hydrolysis half-lives: $t_{1/2} = 3.2$ yr under natural conditions at 30°C, $t_{1/2} = 11.6$ d at 30°C and $t_{1/2} = 25$ d at 18°C and at pH 9 (Howard 1989; selected, Staples et al. 1997);
     first-order hydrolysis $t_{1/2} = 1163$ d based on a second-order rate constant at pH 7 and 30°C; and a base rate constant k = 111.6 M^{-1} h^{-1} corresponding to $t_{1/2} = 1.2$ d at pH 9 and 18°C (Howard et al. 1991)
     $t_{1/2} = 1200$ d at pH 7, $t_{1/2} = 0.026$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: calculated rate constant k = (9.49 ± 0.41) × 10^2 min^{-1} from retention times in reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);
     significant degradation with rapid adaption within 7 d in an aerobic environment with a rate k > 0.5 d^{-1} (Tabak et al. 1981; quoted, Mills et al. 1982);
     biodegradation rate constant k = 1.2 × 10^{-4} mL·cell^{-1}·d^{-1} in river die-away test (Scow 1982);
     58–88% mineralization in 7 d in municipal digested sludge (Horowitz et al. 1982);
     rate constant k = 0.364 d^{-1} which corresponds to $t_{1/2} = 1.90$ d in shake flask biodegradation experiments (Sugatt et al. 1984);
     greater than 90% of DMP was degraded within 40 d in digested sludge (Shelton et al. 1984);
     biodegraded in excess of 90% in activated sludge systems in less than 24 h (O'Grady et al. 1985);
     soil-water biodegradation studies showed that 85% loss in Broome County soil after 120 hours and 75% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with a first-order $k = 8.9 \times 10^{-3}$ h^{-1} and $t_{1/2} = 78$ h (Ziogou et al. 1989);

aqueous aerobic $t_{1/2} = 24$–168 h, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data; aqueous anaerobic $t_{1/2} = 96$–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$(aerobic) = 3 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)

$k = 0.0290$ h^{-1} with $t_{1/2} = 23.9$ h for microbial degradation by anaerobic sludge (Wang et al. 2000)

Aerobic biodegradation in aquatic environments, first order $k = 0.5$ d^{-1} with $t_{1/2} = 1.39$ d in river water, $k = 0.5$ d^{-1} with $t_{1/2} = 1.39$ d in MITI inoculum (Peterson & Staples 2003)

Aerobic biodegradation in soil, pseudo-first-order rate $k = 0.36$ d^{-1} with $t_{1/2} = 1.93$ d in agitated aqueous suspension, and $k = 0.40$ d^{-1} with $t_{1/2} = 1.70$ d at 30°C in garden soil. For anaerobic degradation, first order rate $k = 0.25$–0.696 d^{-1} with $t_{1/2} = 2.8$–1.0 d in digester sludge, batch incubation; $k = 0.033$ d^{-1} with $t_{1/2} = 21$ d in flood soil (Peterson & Staples 2003)

Biotransformation: estimated rate constant $k \sim 5.2 \times 10^{-6}$ mL cell^{-1} h^{-1} for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982).

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

depuration $t_{1/2} = 24$–48 h from bluegill sunfish (Barrows et al. 1980).

$k_2 = 27.7$ d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 2.37$ d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 23.8$ h for reaction with hydroxyl radicals (Howard 1989);

$t_{1/2} = 112$–1118 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

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

$t_{1/2} = 14.41$ d based on photooxidation reaction rate with OH radical, indirect photolysis $t_{1/2} = 14.4$ d (Peterson & Staples 2003)

Surface water: estimated $t_{1/2} < 0.3$ d in river waters (Zoeteman et al. 1980);

mineralization $t_{1/2} \sim 7$ d in municipal digested sludge (Horowitz et al. 1982);

biodegradation $t_{1/2} = 1.90$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

$t_{1/2} < 192$–264 h by biodegradation in fresh river water, $t_{1/2} = 12$ h in Rhine River, an estimated $t_{1/2} \sim 13$–27 h in a modelling study of simulated ecosystem; abiotic degradation $t_{1/2} = 12.7$ h in pure water and $t_{1/2} = 2.8$ h in the presence of nitrogen dioxide when irradiated with a UV lamp (Howard 1989);

overall degradation $t_{1/2} = 24$–168 h, based on unacclimated river die-away test data (Howard et al. 1991)

Biodegradation $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 4 d in natural waters (Capel & Larson 1995)

k(exptl) = (0.20 ± 0.10) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21- 1°C, with $t_{1/2} = 1.9$ d at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 4 d and $t_{1/2} = 1200$ at pH 7, $t_{1/2} = 0.026$ d at pH 12 in natural waters (Capel & Larson 1995)

$t_{1/2} = 0.5$–1.39 d for biodegradation in aerobic aquatic environments (Peterson & Staples 2003)

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

Sediment:

Soil: biodegradation $t_{1/2} < 5$ d (aerobic) and $t_{1/2} \sim 20$ d (anaerobic) in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10$–50 d, via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$t_{1/2} = 24$–168 h, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data (Howard et al. 1991)

Biodegradation in aerobic soil: $t_{1/2} = 1.93$ d in agitated aqueous suspension and $t_{1/2} = 1.70$ d in garden soil (Peterson & Staples 2003)

Biota: $24 < t_{1/2} < 48$ h depuration half-life in tissues of bluefill sunfish in 21 d-exposure experiment (Barrows et al. 1980; quoted, Howard 1989);

$t_{1/2} = 23.9$ h for microbial degradation by anaerobic sludge (Wang et al.2000).

TABLE 15.1.3.1.1
Reported vapor pressures of dimethyl phthalate at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

Gardner & Brewer 1937		Stull 1947	
ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
82.0	40.0	100.3	133.3
85.0	53.3	131.8	666.6
90.0	66.7	147.6	1333
99.0	80.0	164.0	2666
103.0	120	182.8	5333
105.3	160	194.0	7999
107.4	213	210.0	13332
110.6	227	232.7	26664
115.0	267	257.8	53329
118.0	333	283.7	101325
123.8	440		
129.5	587	mp/°C	
136.9	813		
146.5	1293		
146.9	1293		
150.6	1533		
151.0	1547		
bp/°C	140.586		
	at 1 mmHg		
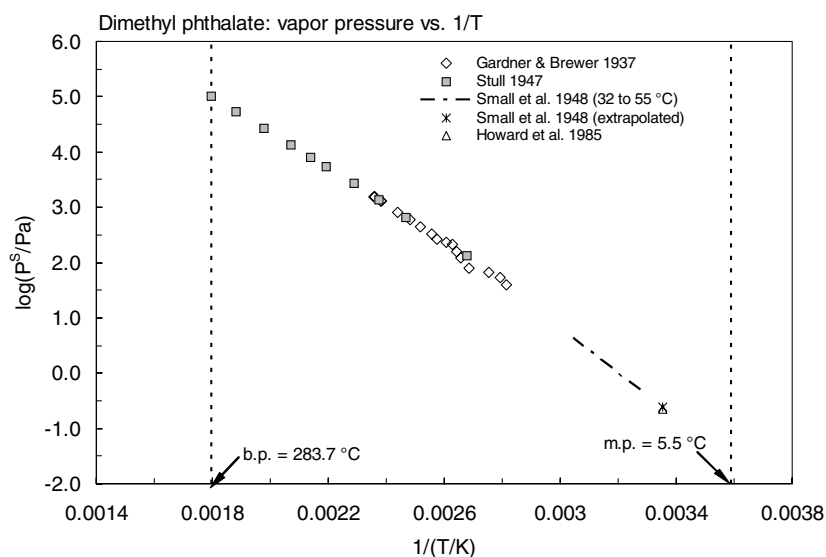
FIGURE 15.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl phthalate.

15.1.3.2   Diethyl phthalate (DEP)
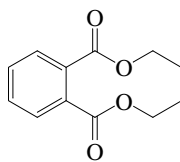
Common Name: Diethyl phthalate
Synonym: DEP, ethyl phthalate
Chemical Name: phthalic acid diethyl ester, ethyl phthalate, 1,2-benzenedicarboxylic acid ethyl ester
CAS Registry No: 84-66-2
Molecular Formula: $C_{12}H_{14}O_4$, $C_6H_4(COOC_2H_5)_2$
Molecular Weight: 222.237
Melting Point (°C):
    –40.5   (Patty 1963; Fishbein & Albro 1972; Lide 2003)
Boiling Point (°C):
    295   (Lide 2003)
Density (g/cm³ at 20°C):
    1.123   (25°C, Fishbein & Albro 1972)
    1.1175   (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
    198.9   (20°C, calculated-density, Stephenson & Malanowski 1987)
    254.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    82.42   (Small et al. 1948)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K) F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are
    compiled at the end of this section):
    598   (Deno & Berkheimer 1960)
    1000   (20°C, Fishbein & Albro 1972)
    1000   (32°C, from Monsanto Chemical Co. data sheets, Peakall 1975)
    896   (shake flask-GC, Wolfe et al. 1980b)
    1200*   (20°C, elution chromatography, UV, Schwarz & Miller 1980)
    7028   (shake flask-LSC, Veith et al. 1980)
    928   (20°C, shake flask-UV, Leyder & Boulanger 1983)
    1080   (shake flask-HPLC/UV, Howard et al. 1985)
    680   (measured, Russell & McDuffie 1986)
    938*   (shake flask-surface tension measurement, measured range 10–35°C Thomsen et al. 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
    temperatures designated * are compiled at the end of this section):
    0.467*   (extrapolated-regression of tabulated data, temp range 108.8–294°C, Stull 1947)
    0.086   (effusion method, extrapolated-Antoine eq., Small et al. 1948)
    log (P/mmHg) = 11.26 – 4308/(T/K); temp range 32–60°C or pressure range 5×10^{-2} to 10^{-4} mmHg (effusion
        method, data presented in graph and Antoine eq., Small et al. 1948)
    0.052   (20°C, torsion-effusion method, Balson 1958)
    0.0195   (20°C, aerosol saturation, measured range 25–70°C, Frostling 1970)
    log (P/mmHg) = 11.13 – 4275/(T/K); temp range 25–70°C (aerosol saturation, Frostling 1970)
    0.467   (calculated-Antoine eq., Weast 1972–73)
    log (P/mmHg) = [–0.2185 × 15383.0/(T/K)] + 8.18275; temp range 108.8–294°C (Antoine eq., Weast 1972–73)

0.046*   (20°C, extrapolated, gas-saturation method, measured range 34.2–60.5°C, Grayson & Fosbraey 1982)

ln (P/Pa) = 32.50 – 10436/(T/K); temp range 34.2–60.5°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)

1.867   (gas saturation, measured range 60–120°C. Potin-Gautier et al. 1982)

log (P/mmHg) = 8.806 – 1443.039/(T/K); temp range 60–120°C (Potin-Gautier et al. 1982)

0.220   (gas saturation-HPLC/UV, Howard et al. 1985)

0.0064   (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.04308 – 1866.05/(–115.9 + T/K); temp range 345–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 10.6902 – 6768.3/(–209.45 + T/K); temp range 421–570 K (Antoine eq.-II, Stephenson & Malanowski 1987)

0.280   (GC-RT correlation, Hinckley et al. 1990)

log (P/mmHg) = 72.1438 – 7.0747 × 10^3/(T/K) – 21.029·log(T/K) – 3.2404 × 10^{-10}·(T/K) + 3.4691 × 10^{-6}·(T/K)^2; temp range 269–757 K (vapor pressure eq., Yaws et al. 1994)

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

0.0020   (calculated-P/C, Wolfe et al. 1980a)

0.0486   (Lyman et al. 1982; quoted, Howard 1989)

0.1220   (calculated-P/C, Mabey et al. 1982)

4.7100   (quoted from WERL Treatability Data, Ryan et al. 1988)

0.0269   (selected, Staples et al. 1997)

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

3.22   (calculated as per Leo et al. 1971)

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

1.40   (shake flask-LSC, Veith et al. 1980)

2.67   (RP-HPLC-RT correlation, Veith et al. 1980)

2.21   (HPLC-RT correlation, McDuffie 1981)

2.70   (quoted from Veith et al. 1980, Veith & Kosian 1983; Davies & Dobbs 1984; Saito et al. 1992)

2.35   (20°C, shake flask-UV, Leyder & Boulanger 1983)

2.24, 2.29   (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)

2.47   (shake flask, unpublished data, Hansch & Leo 1985; 1987)

3.00   (RP-HPLC-RT correlation, De Koch & Lord 1987)

2.47   (recommended, Sangster 1993)

2.47   (recommended, Hansch et al. 1995)

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

7.55   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

0.49–1.56   (calculated-K_{OW}, Veith et al. 1979, 1980)

2.07   (bluegill sunfish, Veith et al. 1980; Barrows et al. 1980; Veith & Kosian 1983)

1.86   (bacteria, calculated-K_{OW}, Wolfe et al. 1980a)

1.08, 1.64   (calculated-S, calculated-K_{OW}, Lyman et al. 1982)

2.04   (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

1.19   (mullet, Shimada et al. 1983)

2.10   (Davies & Dobbs 1984)

2.07   (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

2.65   (calculated-K_{OW}, Wolfe et al. 1980a)

2.72   (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)

1.97   (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

2.15   (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

1.34	(sediment, calculated-K_{OW}, Pavlou & Weston 1983, 1984)
1.84	(Broome County of New York soil, shake flask-GC, Russell & McDuffie 1986)
3.00, 2.85, 3.24	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
2.03	(activated carbon, calculated-MCI χ, Blum et al. 1994)
1.99	(calculated-K_{OW}, Kollig 1993)
1.84	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.84	(sediment/soil, selected, Staples et al. 1997)
4.90	(suspended solids, calculated-K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)

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

Volatilization:

Photolysis: direct $k_P = 2 \times 10^{-4}$ h^{-1} (EXAMS model, Wolfe et al. 1980a)

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

  k(aq.) = 18 M^{-1} s^{-1} in aquatic environment (Wolfe et al. 1980a)

  k << 360 M^{-1} h^{-1} for singlet oxygen and k = 1.4 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)

  $k_{OH} = 1.08 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} corresponding to $t_{1/2}$ = 22.2 h and the alkyl peroxy reaction $t_{1/2}$(calc) = 6.5 yr (Howard 1989)

  photooxidation $t_{1/2}$ = 21–212 h in air, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

  photooxidation $t_{1/2}$ = 2.4–12.2 yr in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Howard et al. 1991)

  k(aq.) = (0.14 ± 0.05) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2}$ = 2.8 d at pH 7 (Yao & Haag 1991).

  k_{OH}(aq.) = 4 × 10^9 M^{-1} s^{-1} for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

  predicted atmospheric photooxidation $t_{1/2}$ = 1.8–18 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

  $k_{OH} = 3.466 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 2.39 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis: k(acid-catalyzed) = 0.04 M^{-1} h^{-1}, k(alkaline) = 79 M^{-1} h^{-1}; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2}$ = 4 months to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

  k(second-order alkaline) = 2.5 × 10^{-2} M^{-1} s^{-1} at 30°C (Wolfe et al. 1980b; quoted, Kollig 1993)

  k(alkaline) = 2.5 × 10^{-2} M^{-1} s^{-1} at 30°C and k (second-order alkaline rate) = 1.2 × 10^{-2} M^{-1} s^{-1} at pH 10–12 at 30°C, with a calculated $t_{1/2}$ = 18.3 yr at pH 7 (Callahan et al. 1979)

  First order hydrolysis $t_{1/2}$ = 8.8 yr based on base rate constant at 30°C and pH 7; base rate constant k = 90 M^{-1} s^{-1} with $t_{1/2}$ = 32 d based on measured rate constant at 30°C and pH from 10 to 12 (Howard et al. 1991)

  $t_{1/2}$ = 3200 d, $t_{1/2}$ = 0.032 d in natural waters (Capel & Larson 1995)

  first-order hydrolysis $t_{1/2}$ = 8.8 yr at pH 7 and $t_{1/2}$ = 32 d at pH 10–12 based on base rate constant at 30°C (Howard et al. 1991; selected, Staples et al. 1997)

Biodegradation: microbial degradation $t_{1/2}$ = 10.5 d by microorganisms isolated from soil and waste water at 30°C (Kurane et al. 1977, quoted, Russell et al. 1985);

  estimated rate constant k ~ (6.59 ± 0.43) × 10^2 min^{-1} from retention times of reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);

  microbial degradation k = 2 × 10^{-4} h^{-1} in an aquatic environment (Wolfe et al. 1980a);

  0 to 32% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

  complete degradation in 7.0 d for 5 and 10 ppm DEP in domestic waste water under aerobic conditions at 25°C (Tabak et al. 1981; quoted, Howard 1989);

  k = 0.315 d^{-1} corresponding to $t_{1/2}$ = 2.21 d with a mixed microbial population and underwent > 99% degradation in 28-d in shake flask biodegradation experiment (Sugatt et al. 1984);

  greater than 90% of DEP was degraded within 40 d in digested sludge (Shelton et al. 1984); 85% biodegraded after 14 d incubation in aerobic freshwater sediments at 22°C (Johnson et al. 1984);

  biodegraded in excess of 90% in less than 24 h in activated sludge systems (O'Grady et al. 1985);

soil-water biodegradation studies showed the 86% loss after 120 h in Broome County soils and 67% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with first-order $k = 6.0 \times 10^{-3}$ h^{-1} and $t_{1/2} = 115$ h (Ziogou et al. 1989)

aqueous aerobic $t_{1/2} = 72–1344$ h, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672–5376$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and anaerobic screening test data (Howard et al. 1991)

$t_{1/2}$(aerobic) = 3 d, $t_{1/2}$(anaerobic) = 28 d in natural waters (Capel & Larson 1995)

Aerobic biodegradation in aquatic environments, first order $k = 1.8$ d^{-1} with $t_{1/2} = 0.39$ d in river water, $k = 0.16$ d^{-1} with $t_{1/2} = 4.33$ d in MITI inoculum, and $k = 0.98$ d^{-1} with $t_{1/2} = 0.71$ d (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 0.38$ d^{-1} with $t_{1/2} = 1.83$ d in agitated aqueous suspension. For anaerobic degradation, first order rate $k = 0.069$ to > 0.3 d^{-1} with $t_{1/2} = 10.0$ to < 2.3 d in digester sludge, batch incubation; $k = 0.036$ d^{-1} with $t_{1/2} = 19.3$ d in flood soil; $k = 0.27$ d^{-1} with $t_{1/2} = 2.6$ d in pond sediment, $k = 0.13$ d^{-1} with $t_{1/2} = 5.3$ d in 10% freshwater sediment and $k = 0.31$ d^{-1} with $t_{1/2} = 2.2$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: experimentally determined microbial $k = 3.2 \times 10^{-9}$ mL organism^{-1} h^{-1} (Wolfe et al. 1980a,c); estimated $k \sim 1 \times 10^{-7}$ mL cell^{-1} h^{-1} for bacterial transformation in water (Mabey et al. 1982); mean microbial $k = (7.2 \pm 15.4) \times 10^{-7}$ mL cell^{-1} h^{-1} for 54 batch aufwuchs cultures (Lewis & Holm 1981; Lewis et al. 1984).

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

depuration half-life 24 h $< t_{1/2} < 48$ h in tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 6.83$ d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.584$ d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: an estimated $t_{1/2} = 22.2$ h for the vapor reaction with photochemically generated 8×10^5 molecules·cm^{-3} OH radical in air at 25°C with an estimated $k \sim 1.08 \times 10^{-11}$ cm^3·molecule^{-1}·s^{-1} (Howard 1989);

$t_{1/2} = 21–212$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photodegradation $t_{1/2} = 2.39$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 2.21$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984); $t_{1/2} \sim 2$ d to > 2 wk for aerobic biodegradation in water; $t_{1/2} = 3$ d when incubated in dirty river water (Howard 1989);

overall degradation $t_{1/2} = 72–1344$ h, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991);

k(exptl) = (0.14 ± 0.5) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 2.8$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 144–2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 14$ d in freshwater sediment (Johnson et al. 1984).

Soil: degradation $t_{1/2} = 10.5$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977); $t_{1/2} = 10–50$ d via volatilization subject to plant uptake from soil (Ryan et al. 1988); $t_{1/2} = 72–1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: 24 h $< t_{1/2} < 48$ h in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 15.1.3.2.1
Reported vapor pressures and aqueous solubilities of diethyl phthalate at various pressures and solubilities

Aqueous solubility				Vapor pressure			
Schwarz & Miller 1980		Thomsen et al. 2001		Stull 1947		Grayson & Fosbraey 1982	
elution chromatography-UV		shake flask-surface tension		summary of literature data		gas saturation-GC	
t/°C	g m⁻³	t/°C	g m⁻³	t/°C	P/Pa	t/°C	P/Pa
20	1200	10	1113	108.8	133.3	34.2	0.222
20	1240	25	838	140.7	666.6	40.0	0.470
20	1160	35	741	156.0	1333	44.8	0.784
30	1370			173.6	2666	50.7	1.368
30	1400			192.1	5333	60.5	3.320
30	1340			204.1	7999	20	0.046
				219.5	13332		
				243.0	26664	$\ln P = A - B/(T/K)$	
				267.5	53329		P/Pa
				294.0	101325	A	32.5
						B	10436

Diethyl phthalate: solubility vs. 1/T

◇ Thomsen et al. 2001 (see text for data)
✳ Wolfe et al. 1980b
△ Veith et al. 1980
✕ Leyder & Boulanger 1983
□ Howard et al. 1985
○ Russell & McDuffie 1986
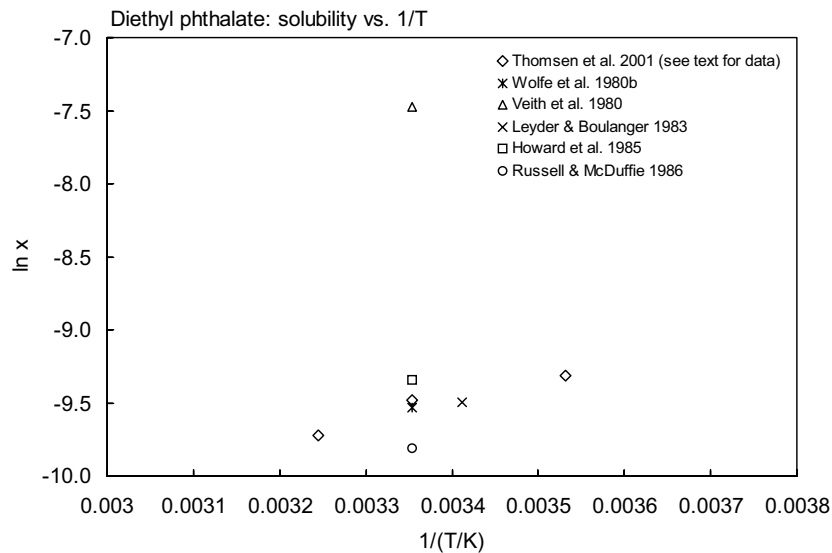
FIGURE 15.1.3.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for diethyl phthalate.

Diethyl phthalate: vapor pressure vs. 1/T
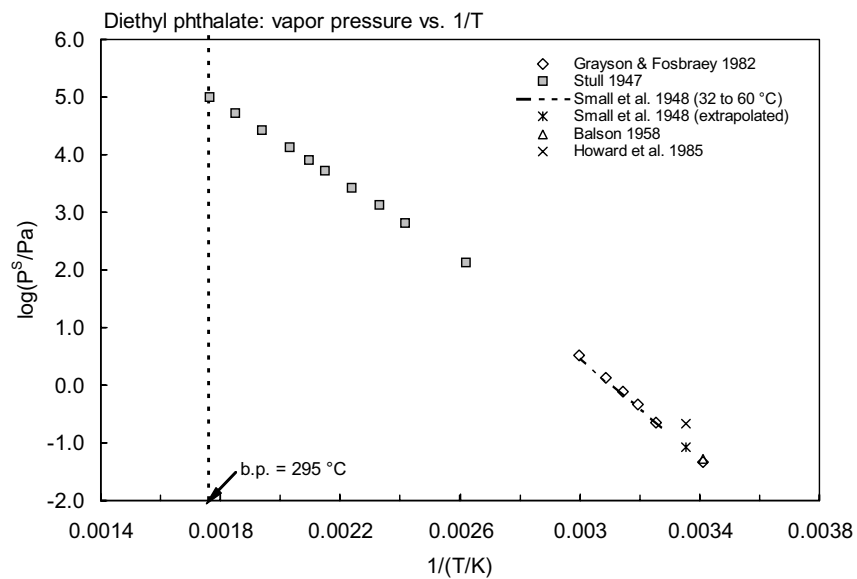
FIGURE 15.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl phthalate.

15.1.3.3   Diallyl phthalate (DAP)
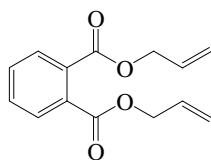
Common Name: Diallyl phthalate
Synonym: DAP
Chemical Name: di(2-propenyl) phthalate, bis(2-propenyl)ester, 1,2-benzenedicarboxylic acid
CAS Registry No: 131-17-9
Molecular Formula: $C_{14}H_{14}O_4$, C_6H_4-1,2-$(CO_2CH_2CH{=}CH_2)_2$
Molecular Weight: 246.259
Melting Point (°C):
    –77   (Fishbein & Albro 1972)
Boiling Point (°C):
    290   (Fishbein & Albro 1972)
Density (g/cm³ at 20°C):
    1.121   (Fishbein & Albro 1972)
Molar Volume (cm³/mol):
    219.7   (20°C, calculated-density)
    288.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
    < 100   (Fishbein & Albro 1972)
    182   (20°C, shake flask-GC, Leyder & Boulanger 1983)
    182; 43, 100 (recommended; calculated-QSAR, Staples 1997)
    94   (calculated-UNIFAC, Thomsen et al. 1999)
    156   (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
    0.0213; 0.00493, 0.155   (recommended; calculated-QSAR, Staples et al. 1997)
    0.0271   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.0289   (selected, Staples et al. 1997)
    0.0428   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    3.23   (shake flask, Leyder & Boulanger 1983)
    3.23   (recommended value, Sangster 1993)
    3.23   (recommended, Hansch et al. 1995)
    3.23; 3.37, 3.63   (recommended; calculated-QSAR, Staples 1997)
    3.61   (calculated-UNIFAC, Thomsen et al. 1999)
    3.11   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    7.87   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: atmospheric photooxidation $t_{1/2}$ = 0.04–0.4 d (Staples et al. 1997).
    Hydrolysis:
    Biodegradation: degradation $t_{1/2}$ = 2.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste
        water at 30°C (Kurane et al. 1977).
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
    Air: atmospheric photooxidation $t_{1/2}$ = 0.04–0.4 d (Staples et al. 1997).
    Surface water:
    Groundwater:
    Sediment:
    Soil: degradation $t_{1/2}$ = 2.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at
        30°C (Kurane et al. 1977).
    Biota:

15.1.3.4   Di-*n*-propyl phthalate (DnPP)
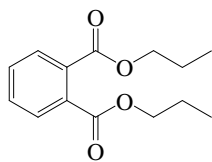
Common Name: Di-*n*-propyl phthalate
Synonym: DPP, DNPP, dipropyl phthalate
Chemical Name: phthalic acid dipropyl ester; 1,2-benzenedicarboxylic acid dipropyl ester
CAS Registry No: 131-16-8
Molecular Formula: $C_{14}H_{18}O_4$, $C_6H_4[COOCH_2CH_2CH_3]_2$
Molecular Weight: 250.291
Melting Point (°C):
    –31.0   (Lide 2003)
Boiling Point (°C):
    304.5   (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
    232.2   (20°C, calculated-density, Stephenson & Malanowski 1987)
    302.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    88.70   (Small et al. 1948)
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):
    108   (shake flask-UV, Leyder & Boulanger 1983)
    108; 38, 47 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)
    77   (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    0.0175   (effusion method, extrapolated-Antoine eq., Small et al. 1948)
    log (P/mmHg) = 11.66 – 4634/(T/K); temp range 32–75°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine
        eq., effusion method, Small et al. 1948). Additional data at other temperatures designated * are compiled
        at the end of this section
    log (P/kPa) = 8.625 – 3824/(T/K); temp range 403–578 K (Antoine eq., Stephenson & Malanowski 1987)
    0.0119, 0.138   (calculated-QSAR, Staples et al. 1997)
    0.0175   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.0309   (recommended, Staples et al. 1997)
    0.0569   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    3.27   (shake flask, Leyder & Boulanger 1983)
    4.05   (HPLC-RT correlation, Hayward et al. 1990)
    4.20   (HPLC-RT correlation, Jenke et al. 1990)
    3,27, 4.05   (lit. values, Hansch et al. 1995)
    3.27; 3.57, 3.63   (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)
    3.636   (Thomsen & Carlsen 1998)
    3.40   (calculated-QSPR, Cousins & Mackay 2000)

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

    8.04   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:

    Photolysis:

    Oxidation: atmospheric photooxidation $t_{1/2}$ = 0.9–9.0 d (calculated, Staples et al. 1997).

    Hydrolysis:

    Biodegradation: degradation $t_{1/2}$ = 6.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste
        water at 30°C (Kurane et al. 1977);

        rate constant k = $(10.71 \pm 0.73) \times 10^{-2}$ min^{-1} was estimated from the retention time in reverse phase
            chromatography (Urushigawa & Yonezawa 1979).

        Aerobic biodegradation in aquatic environments, first order k = 1.3 d^{-1} with $t_{1/2}$ = 0.53 d in river water
            (Peterson & Staples 2003)

    Biotransformation:

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

Half-Lives in the Environment:

    Air: atmospheric photooxidation $t_{1/2}$ = 0.9–9.0 d (calculated, Staples et al. 1997).

    Surface water: $t_{1/2}$ = 0.53 d in river water (Peterson & Staples 2003)

    Groundwater:

    Sediment:

    Soil: degradation $t_{1/2}$ = 6.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at
        30°C (Kurane et al. 1977).

    Biota:
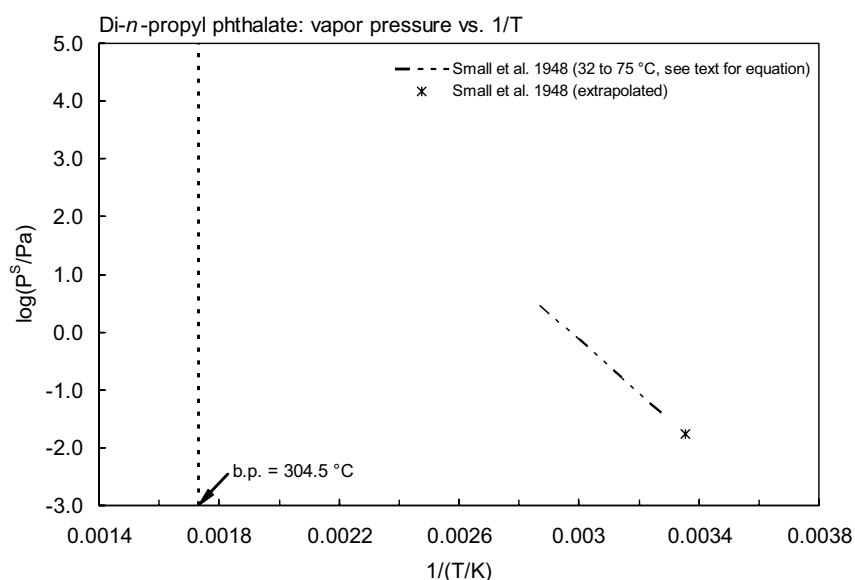
FIGURE 15.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl phthalate.

15.1.3.5   Di-isopropyl phthalate (DIPP)
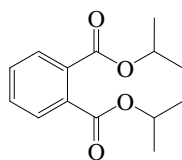
Common Name: Di-isopropyl phthalate
Synonym: DIPP
Chemical Name: phthalic acid dipropyl ester, bis(1-methylethyl)ester, 1,2-benzenedicarboxylic acid didiopropy ester
CAS Registry No: 605-45-8
Molecular Formula: $C_{14}H_{18}O_4$, 1,2-$C_6H_4(CO_2C_3H_7)_2$
Molecular Weight: 250.291
Melting Point (°C): liquid
Boiling Point (°C):
    304–305 (Weast 1982–83)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
    302.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    322   (shake flask-UV, Leyder & Boulanger 1983)
    136   (calculated-UNIFAC, Thomsen et al. 1999)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
    2.83   (shake flask-UV, Leyder & Boulanger 1983)
    2.83   (recommended, Sangster 1993)
    2.83   (recommended, Hansch et al. 1995)
    3.59   (calculated-UNIFAC, Thomsen et al. 1999)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{\frac{1}{2}}$:
    Biodegradation: degradation $t_{\frac{1}{2}}$ = 1.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste
        water at 30°C (Kurane et al. 1977).

Half-Lives in the Environment:
    Soil: degradation $t_{\frac{1}{2}}$ = 1.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at
        30°C (Kurane et al. 1977).

15.1.3.6   Di-*n*-butyl phthalate (DBP)
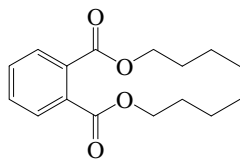
Common Name: Dibutyl phthalate
Synonym: *n*-butyl phthalate, di-*n*-butyl phthalate, DBP, dibutyl *o*-phthalate, *o*-benzenedicarboxylic acid dibutyl ester, benzene-*o*-dicarboxylic acid dibutyl ester
Chemical Name: phthalic acid dibutyl ester, di-*n*-butyl phthalate
CAS Registry No: 84-74-2
Molecular Formula: $C_{16}H_{22}O_4$, o-$C_6H_4(COOC_4H_9)_2$
Molecular Weight: 278.344
Melting Point (°C):
    –35.0   (Fishbein & Albro 1972; Verschueren 1977, 1983; Dean 1985; Howard 1989; Lide 2003)
Boiling Point (°C):
    340.0   (Stull 1947; Fishbein & Albro 1972; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
    1.0465   (21°C, Fishbein & Albro 1972)
    1.047   (Weast 1982–83)
Molar Volume (cm³/mol):
    267.1   (calculated-density, Stephenson & Malanowski 1987)
    347.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    93.3   (Small et al. 1948)
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):
    11.08   (Deno & Berkheimer 1960)
    4500   (Patty 1967)
    4500   (Fishbein & Albro 1972)
    10.0   (30°C, from Monsanto Chemical Co. data sheets, Peakall 1975)
    13.0   (Wolfe et al. 1979; Wolfe et al. 1980a)
    10.8, 11.1, 10.5 (20°C: quoted average, elution chromatography, UV, Schwarz & Miller 1980)
    11.4, 11.5, 11.2 (30°C: quoted average, elution chromatography, UV, Schwarz & Miller 1980)
    13 ± 1.6, 4.45   (shake flask-GC, quoted, Wolfe et al. 1980b; quoted, Staples et al. 1997)
    3.25   (solubility in 35 liter instant ocean, Giam et al. 1980)
   10.1   (20°C, shake flask-UV, Leyder & Boulanger 1983)
    400, 4500   (Verschueren 1983)
    28.0   (26°C, Verschueren 1983)
    11.2 ± 0.3   (shake flask-HPLC/UV, Howard et al. 1985)
    100   (Dean 1985)
    11.2   (Howard et al. 1985)
    9.40   (best estimate by turbidity inflection, DeFoe et al. 1990)
    8.70, 9.40   (centrifugation-HPLC/UV, turbidity inflection-HPLC/UV, DeFoe et al. 1990)
    11.2   (recommended, Staples et al. 1997)
    9.90   (calculated-QSPR, Cousin & Mackay 2000)
    13.3, 14.6, 5.50 (10, 25, 35°C, shake flask-surface tension measurement, Thomsen et al. 2001). Additional
        data at other temperatures designated * are compiled at the end of this section

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*   (89°C, ebulliometry, measured range 89–176°C, Gardner & Brewer 1937)

0.00233   (20°C, extrapolated, tensimeter, measured range 52–97°C, Hickman et al. 1937)

$\log (P/\mu\text{mHg}) = 14.215 - 4680/(T/K)$; temp range 52–97°C (Hickman et al. 1937)

0.0171*   (20°C, extrapolated, effusion, measured range 40–95°C, Verhoek & Marshall 1939)

$\log (P/\mu\text{mHg}) = 15.589 - 5122/(T/K)$; temp range 40–95°C (Verhoek & Marshall 1939)

0.00253*   (ebulliometry, extrapolated from graph, measured range 50–172°C, Burrows 1946)

0.0217*   (extrapolated-regression of tabulated data, temp range 148.2–340°C, Stull 1947)

0.00345, 0.0043   (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log (P/\text{mmHg}) = 11.75 - 4871/(T/K)$; temp range ~ 32–75°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, Small et al. 1948)

$\log (P/\text{mmHg}) = 11.86 - 4875/(T/K)$; temp range ~ 40–95°C or pressure range 5×10^{-2} to 10^{-4} mmHg (redistilled technical grade, Antoine eq., effusion method, Small et al. 1948)

0.00276   (extrapolated-combined vapor pressure eq., Small et al. 1948)

$\log (P/\text{mmHg}) = 7.065 - 1666/(T/K) - 547700/(T/K)^2$; temp range ~ 35–352°C (combined vapor pressure eq. derived from effusion measurement results and other published data, Small et al. 1948)

0.0033   (20°C, extrapolated, tensimeter, measured range 55–102°C, Perry & Weber 1949)

$\log (P/\mu\text{mHg}) = 13.58 - 4450/(T/K)$; temp range 55–102°C (pendulum-tensimeter method, Perry & Weber 1949)

0.00364*   (effusion method, measured range 19.9–44°C, Birks & Bradley 1949)

7.6×10^{-5} (dew-point method and tensimeter method, temp range of 72–185°C, extrapolated-Antoine eq., Werner 1952)

$\log (P/\mu\text{mHg}) = 11.008 - 2872/(176.5 + t/°C)$; temp range 72–185°C (Antoine eq., dew-point method and tensimeter method, Werner 1952)

32*   (125.7°C, vapor-liquid equilibrium data, measured range 125.7–202.5°C, Hammer & Lydersen 1957)

$\log (P/\text{kPa}) = 6.439 - 1011/(T/K) - 720000/(T/K)^2$; temp range 125.7–202.5°C, Hammer & Lydersen 1957)

1.53*   (86.5°C, transpiration method, measured range 86.5–144°C, Franck 1969)

$\log (P/\text{mmHg}) = [-0.2185 \times 17747.0/(T/K)] + 9.217428$; temp range: 148.2–340°C, (Antoine eq., Weast 1972–73)

3.87×10^{-4} (6.55°C, submicron droplet evaporation, measured range 6.55–12.55°C, Ray et al. 1979)

$\log (P/\text{mmHg}) = 12.217 - 4993/(T/K)$; temp range 6.55–12.55°C (submicron droplet evaporation, Ray et al. 1979)

0.00206*   (20°C, transpiration-GC "collection" measurement, Hales et al. 1981)

$\ln (P/\text{Pa}) = 27.5178 - 8739.43/(T/K) - 330691/(T/K)^2$; temp range 293–373 K (empirical vapor pressure eq., from transpiration-GC measurement, Hales et al. 1981)

0.0023*   (20°C, vapor pressure balance, temp range 10–50°C, OECD 1981)

0.00277   (20°C, evaporation rate-gravimetric method, Gückel et al. 1982)

0.00133   (gas saturation, Jaber et al. 1982)

0.40, 0.0653, 1.0   (structure-based estimation methods, Tucker et al. 1983)

1.55×10^{-4} (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 576561 - 1744.128/(188.880 + t/°C)$, temp range 125.8–202.5°C (Antoine eq. derived from exptl. data of Hammer & Lydersen 1957, Boublik et al. 1984)

0.00230   (OECD 1981 Guidelines, Dobbs et al. 1984)

0.0011   (saturated column-HPLC/UV, Howard et al. 1985)

0.00355   (extrapolated, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.8788 - 2538.4/(-92.25 + T/K)$; temp range 314–469 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.97157 - 3385.9/(-37.18 + T/K)$; temp range 468–605 K (Antoine eq.-II, Stephenson & Malanowski 1987)

0.0244   (calculated-solvatochromic parameters, Banerjee et al. 1990)

0.0056   (GC-RT correlation, Hinckley et al. 1990)

$\log (P/\text{mmHg}) = 6.63980 - 1744.20/(113.69 + t/°C)$, temp range 126–202°C (Antoine eq., 1992)

$\log (P/\text{mmHg}) = 152.675 - 1.0754 \times 10^4/(T/K) - 51.17 \cdot \log(T/K) + 1.6933 \times 10^{-2} \cdot (T/K) + 2.4948 \times 10^{-14} \cdot (T/K)^2$; temp range 238–781 K (vapor pressure eq., Yaws et al. 1994)

0.0027   (liquid P_L, GC-RT correlation, Donovan 1996)

0.0036   (recommended, Staples et al. 1997)
0.0473   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.1320   (calculated-P/C, Wolfe et al. 1980a)
0.0466   (Lyman et al. 1982; quoted, Howard 1989)
0.0284   (calculated-P/C, Mabey et al. 1982)
0.1835   (Atlas et al. 1983)
0.456, 0.446 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
0.0297   (quoted from WERL Treatability Data, Ryan et al. 1988)
0.0895   (selected, Staples et al. 1997)
0.133   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
5.20   (calculated as per Leo et al. 1971, Callahan et al. 1979)
5.15   (RP-HPLC-RT correlation, Veith et al. 1979)
4.13   (HPLC-RT correlation;, McDuffie 1981)
4.11, range 3.23–4.45   (shake flask-concn ratio, OECD 1981)
4.08   (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
4.39, 4.56 (HPLC-extrapolated, Harnish et al. 1983)
4.57   (20°C, shake flask-UV, Leyder & Boulanger 1983)
4.79, 3.74 (shake flask-HPLC/UV, HPLC-RT, Howard et al. 1985)
4.11   (OECD value, Howard et al. 1985)
4.72   (shake flask, Hansch & Leo 1985; 1987)
4.57   (HPLC-k′ correlation, Eadsforth 1986)
4.30   (HPLC-RT correlation, Haky & Leja 1986)
4.72   (measured value, DeFoe et al. 1990)
4.72   (recommended, Sangster 1993)
4.72   (recommended, Hansch et al. 1993)
4.01   (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)

Octanol/Air Partition Coefficient, log K_{OA}:
8.54   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:
3.15   (fish, Mayer & Sanders 1973)
3.82, 3.70, 3.83, 3.28, 3.70, 3.43   (midge larvae, waterflea, scud, mayfly, grass shrimp, damselfly, Sanders et al. 1973)
3.83   (fish, Sanders et al. 1973)
1.32   (calculated, Kenaga 1980)
3.90   (bacteria, calculated-K_{OW}, Wolfe et al. 1980a)
1.32–1.62, 0.46–1.49, 1.07   (oyster, shrimp, fish, Wofford et al. 1981)
1.50, 1.22, 1.07   (American oyster, brown shrimp, sheephead minnow, Wofford et al. 1981)
4.67   (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
4.36   (*Selenastrum capricornutum*, Casserly et al. 1983)
1.32   (oyster, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
3.68, 3.68 (oyster, estimated values, Zaroogian et al. 1985)
1.08   (fish, highest BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.20   (soil, estimated-S, Kenaga 1980)
3.81   (soil, estimated-S, Wolfe et al. 1980a)
2.17   (marine sediment/seawater with 1% organic carbon, Bouwer et al. 1981)
1.60, 1.30, 0.602   (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 3–4 ppm, Sullivan et al. 1981)

0.301, 0.602, 1.556 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 20 ppb, Sullivan et al. 1981)

5.23 (sediment-water, calculated-K_{OW}, Mabey et al. 1982).

4.17 (sediment/soil, Sullivan et al. 1982; selected, Staples et al. 1997)

4.54 (sediment, calculated-K_{OW}, Pavlou & Weston 1983,84)

3.14 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986)

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

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

3.09, 5.20 (suspended solids, calculated-K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)

3.14; 3.76, 2.46, 2.86, 3.09, 3.12, 3.11 (quoted lit.; values obtained from HPLC-k′ correlation on different stationary phases, Szabo et al. 1999)

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

Volatilization: $t_{1/2}$ = 28 d from a stirred seawater solution 1.0 m deep (Atlas et al. 1982; quoted, Howard 1989) evaporation rate k = 3.42×10^{-10} mol cm^{-2} h^{-1} at 20°C (Gückel et al. 1982);

$t_{1/2}$ ~ 47 d in a river of 1.0 m deep with 1 m/s current and a 3 m/s wind using Henry's law constant while the rate of volatilization being controlled by the diffusion through air (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: direct photolysis (near surface) rate constant k ~ 2×10^{-4} h^{-1} in natural water (Wolfe et al. 1980a) aqueous photolysis rate k = 0.23 h^{-1} and $t_{1/2}$ = 3 h (Jin et al. 1999, quoted, Peterson & Staples 2003) Indirect photolysis k = 0.29 d^{-1} with $t_{1/2}$ = 2.4 d in air (Peterson & Staples 2003).

Oxidation:

k = 18 M s^{-1}, the free radical oxidation rate constant (EXAMS model, Wolfe et al. 1980a)

photooxidation $t_{1/2}$ = 2.4–12.2 yr in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Wolfe et al. 1980a; quoted, Howard et al. 1991)

k << 360 M^{-1} h^{-1} for singlet oxygen and k = 1.4 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2}$ = 18.4 h with reaction with OH radical (Howard 1989)

photooxidation $t_{1/2}$ = 7.4–74 h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Atmospheric photooxidation $t_{1/2}$ = 0.6–6.0 d from Atkinson 1988 atmospheric-oxidation program (estimated, Staples et al. 1997).

k_{OH} = 9.277×10^{-12} cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.89 d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis:

k(second-order alkaline) = 2.2×10^{-2} M^{-1} s^{-1} for pH 10–12 at 30°C, with calculated half-life of 10 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)

k(acid catalyzed) = 0.04 M^{-1} h^{-1}, k(second order alkaline) = 38 M^{-1} h^{-1} in an aquatic environment (Wolfe et al. 1980a)

k(second-order alkaline) = $(1.0 \pm 0.05) \times 10^{-2}$ M^{-1} s^{-1} at pH 7 and 30°C, with first-order hydrolysis $t_{1/2}$ = 10 yr (Wolfe et al. 1980b; quoted, Kollig 1993);

$t_{1/2}$ = 76 d at pH 9 and $t_{1/2}$ = 10 yr at neutral pH (estimated, Howard 1989)

$t_{1/2}$ = 10 yr, based on the overall hydrolysis rate constant (Howard et al. 1991)

aqueous abiotic $t_{1/2}$ = 22 yr (selected, Staples et al. 1997)

$t_{1/2}$ = 3700 d at pH 7, $t_{1/2}$ = 76 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation:

$t_{1/2}$ = 3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

DBP was rapidly degraded, 3% left after 5 d, but under anaerobic conditions required 30 d for the degradation freshwater hydrosoil, under aerobic conditions (Johnson et al. 1979, quoted, Russell et al 1985)

a 90% loss in 3 d from river water (Brinkman et al. 1979, quoted, Russell et al. 1985)

k = $(13.26 \pm 0.73) \times 10^2$ min^{-1} (reversed phase-GC-RT correlation, Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985)

k = 2.9×10^{-8} mL organism^{-1} h^{-1} (Wolfe et al. 1980a);

k > 0.5 d^{-1}, significant degradation with rapid adaptation within 7 d in an aerobic environment (Tabak et al. 1981; quoted, Mills et al. 1982);

k = 7.4×10^{-7} mL cell^{-1} d^{-1} (river die-away test, Scow 1982);

32–85% degraded after 2–3 wk in municipal digested sludge (Horowitz et al. 1982)

decomposed within 80 d under both aerobic and anaerobic conditions when approximately 90% added to soils (Inman et al. 1984)

$k = (0.1–7.6) \times 10^{-4}$ h^{-1} to $(4.9–36.5) \times 10^{-4}$ h^{-1} for water and water/sediment systems (under sterile conditions); and $k = (29.3–409) \times 10^{-4}$ h^{-1} to $(38.2–456) \times 10^{-4}$ h^{-1} for water and water/sediment systems (under active conditions) samples from six estuarine and freshwater sites, actual $t_{1/2} = 1.0–4.8$ d for active sediment treatment, $t_{1/2} = 1.7–13.0$ d for active water treatment and $t_{1/2} = 8–23$ d for sterile sediment (Walker et al. 1984)

$k = 0.050$ d^{-1} and a $t_{1/2} = 15.4$ d in a shake flask biodegradation experiment (Sugatt et al. 1984)

> 90% of DBP was degraded within 40 d in digested sludge (Shelton et al. 1984)

> 90% biodegraded in less than 24 h in activated sludge systems (O'Grady et al. 1985)

81% loss in Broome County soils after 24 h and 70% loss in leachate sprayed soil after 24 h in soil-water biodegradation studies (Russell et al. 1985);

$k = 10.6 \times 10^{-3}$ h^{-1} and $t_{1/2} = 65$ h, anaerobic digestion of sludge (Ziogou et al. 1989);

$t_{1/2} < 5$ d, aerobic conditions, $t_{1/2} = 20$ d under anaerobic conditions in a garden soil (Shanker et al. 1985)

$t_{1/2} = 24–552$ h, aqueous aerobic based on unacclimated aerobic river die-away test and soil grab sample data (Howard et al. 1991);

$t_{1/2} = 48–552$ h, aqueous anaerobic, based on unacclimated anaerobic grab sample data for soil and sediment (Johnson & Lulves 1975; Verschueren 1983; Howard et al. 1991)

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

$k = 0.0216$ h^{-1} with $t_{1/2} = 32.1$ h for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.8$ d^{-1} with $t_{1/2} = 0.87$ d in river water, $k = 0.51$ d^{-1} with $t_{1/2} = 1.56$ d in estuarine and river water, $k = 0.29$ d^{-1} with $t_{1/2} = 2.40$ d in sediment microcosm, $k = 0.22$ d^{-1} with $t_{1/2} = 3.15$ d in MITI inoculum, $k = 0.14$ d^{-1} with $t_{1/2} = 4.95$ d in river water, low sediment, and $k = 0.98$ d^{-1} with $t_{1/2} = 0.71$ d river water only (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 1.61$ d^{-1} with $t_{1/2} = 0.43$ d in agitated aqueous suspension, $k = 0.39$ d^{-1} with $t_{1/2} = 1.8$ d at 30°C garden soil; $k = 0.103$ d^{-1} with $t_{1/2} = 6.7$ d in soil with 2% OC; $k = 0.044$ d^{-1} with $t_{1/2} = 11.2$ d in soil with 3.3% OC and $k = 0.62$ d^{-1} with $t_{1/2} = 15.8$ d in soil with 1.6% OC. For anaerobic degradation, first order rate $k = 0.26–0.581$ d^{-1} with $t_{1/2} = 1.19–2.7$ d in undiluted digester sludge, $k = 0.025–0.073$ d^{-1} with $t_{1/2} = 27.7–9.5$ d in 10% diluted sludge, batch incubation; $k = 0.076$ d^{-1} with $t_{1/2} = 9\ 1$ d in 10% freshwater sediment and $k = 0.051$ d^{-1} with $t_{1/2} = 13\ 6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: $k = (1.9–4.4) \times 10^{-8}$ mL cell^{-1} h^{-1} for bacterial transformation in water (Steen et al. 1979; quoted, Mabey et al. 1982; Steen 1991);

$k = 2.9 \times 10^{-8}$ mL cell^{-1} h^{-1} for bacterial transformation in water (Wolfe et al. 1980a).

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

$t_{1/2} = 3$ d in *Daphnia magna* (Mayer & Sanders 1973).

$k_2 = 0.237$ d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.0114$ d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 18$ h for the vapor phase reaction with hydroxyl radicals in air (Howard 1989);

$t_{1/2} = 7.4–74$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

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

Photodegradation $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air and indirect photolysis $t_{1/2} = 2.4$ d (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 15.4$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984)

$t_{1/2} = 2–12$ d in water alone (Howard 1989);

$t_{1/2} = 24–336$ h, based on unacclimated aerobic river die-away test and fresh water/sediment grab sample data (Howard et al. 1991)

Biodegradation $t_{1/2}$(aerobic) = 1 d, $t_{1/2}$(anaerobic) = 2 d; hydrolysis $t_{1/2} = 3700$ d at pH 7 and $t_{1/2} = 76$ d at pH 12 in natural waters (Capel & Larson 1995)

biodegradation $t_{1/2} = 0.87–5.78$ d in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2}$ = 48–552 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: 97% degradation in 5 d in an aerobic pond water-sediment mixture; $t_{1/2}$ = 7–30 d under anaerobic conditions, $t_{1/2}$ = 1–5 d in sediment-water systems of estuarine and freshwater sites (Howard 1989).

Soil: degradation $t_{1/2}$ = 3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
degradation $t_{1/2}$ = 11 to 53 d as affected by soil type, pH, temperature, aeration status and sterilization (Inman et al. 1984);
biodegradation $t_{1/2}$(aerobic) < 5 d and $t_{1/2}$(anaerobic) ~ 20 d in a garden soil (Shanker et al. 1985);
$t_{1/2}$ = 10–50 d via volatilization subject to plant uptake from soil (Ryan et al. 1988);
overall $t_{1/2}$ = 48–552 h, based on unacclimated aerobic soil grab sample data (Howard et al. 1991)
Aerobic biodegradation in soil, $t_{1/2}$ ranging from 0.43 to 19.8 d in aqueous suspension, garden soil and soils with different organic carbon contents (Peterson & Staples 2003)

Biota: elimination $t_{1/2}$ = 3 d for waterfleas *Daphnia magna* (Mayer & Sanders 1973).
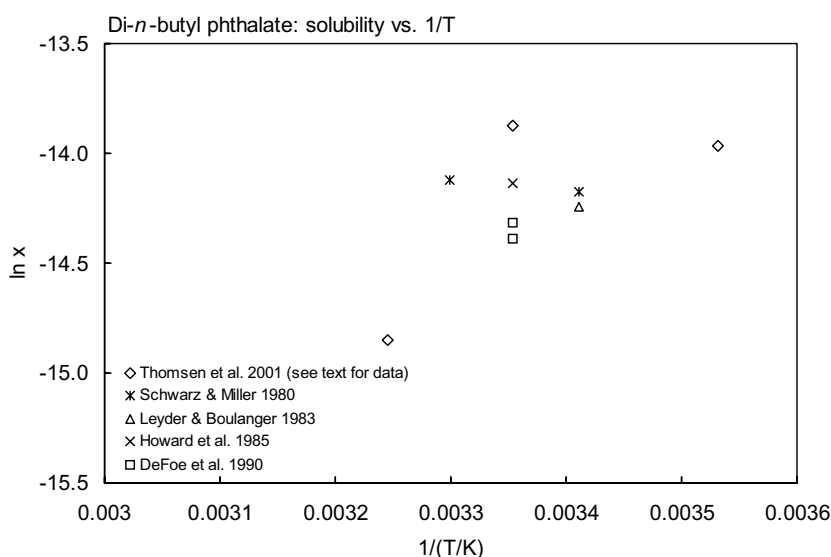
FIGURE 15.1.3.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for di-*n*-butyl phthalate.

TABLE 15.1.3.6.1
Reported vapor pressures of di-*n*-butyl phthalate 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/(T/K)²	(5)	ln P = A – B/(T/K) – C/(T/K)²	(5a)

1.

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
89.0	13.33	40	0.0223	50	0.0667	148.2	133.3
98.8	53.33	55	0.137	82	1.333	182.1	666.6
106.1	79.99	55	0.109	120	26.66	198.2	1333

TABLE 15.1.3.6.1 (*Continued*)

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
111.3	106.7	59.7	0.237	147	133.3	216.2	2666
122.5	120.0	64.7	0.393	172	533.3	235.8	5333
132.0	133.3	65.0	0.409	25	0.00253*	247.8	7999
134.5	120.0	69.7	0.612		*extrapolated	263.7	13332
137.2	133.32	70.0	0.601			287.0	26664
138.0	133.32	74.6	0.981			313.5	53329
141.0	146.7	75.0	1.076			340.0	101325
141.2	146.7	75.0	0.904				
144.8	160.0	85.0	2.880			mp/°C	–
145.4	146.7	85.0	2.520				
147.5	173.3	85.0	2.520				
148.0	160.0	95.0	6.040				
149.5	173.3						
150.0	186.7						
151.0	173.3	eq. 1	P/microns				
153.5	200.0	A	15.589				
162.9	280.0	B	5122				
164.4	293.3						
167.2	373.3	ΔH_V = 98.07 kJ/mol					
168.0	373.3						
168.6	386.6						
171.8	426.6						
176.3	546.6						
bp/°C	340.7						

2.

Small et al. 1948		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
exptl data presented in graph		19.9	0.001907	125.7	32.0	86.5	1.53
		23.0	0.002733	131.55	49.06	86.5	1.63
eq. 2	P/mmHg	25.0	0.003640	139.21	73.86	86.5	1.76
A	11.75	30.0	0.006666	147.02	120	105.5	9.42
B	4871	35	0.01180	156.70	205	105.6	9.88
measured pressure range:		40	0.02106	158.89	228	105.5	10.5
0.05 to 0.001 mmHg		43	0.02933	162.12	277	125.5	37.8
ΔH_V = 93.30 kJ/mol		43.5	0.02959	172.76	480	125.5	36.9
		44	0.03346	180.18	671	125.5	34.9
for redistilled tech. grade				180.36	667	144.5	136.0
eq. 2	P/mmHg	eq. 2	P/mmHg	186.87	921	144.5	109.0
A	11.86	A		195.88	1353	144.5	103.0
B	4875	B		202.05	1739		
ΔH_V = 93.30 kJ/mol		C					

(*Continued*)

TABLE 15.1.3.6.1 (*Continued*)

Small et al. 1947		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				eq. 5	P/kPa	**OECD 1981**	
				A	6.439	**vapor pressure balance**	
Werner 1952				B	1011	t/°C	P/Pa
dew-point/tensimeter method				C	720000	10	6.5×10^{-4}
t/°C	P/Pa					20	2.3×10^{-3}
				In Boublik et al. 1984		30	7.8×10^{-3}
exptl data presented in graph				A	5.76561	40	2.4×10^{-2}
				B	1744.128	50	7.0×10^{-2}
eq. 2	P/mmHg			C	113.731		
A	11.008			bp/°C	188.880		
B	2872						
C	176.5						
temp range: 70–170°C							

3.

Hales et al. 1981

transpiration-GC analysis

t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
collection		continued		continued		overall best fit equation:	
39.89	0.02398	80.02	1.162	19.90	2.064×10^{-3}	eq. 5a	P/Pa
39.92	0.02333	79.95	1.089	20.0	2.065×10^{-3}	A	21.5178
39.92	0.02273	99.93	5.335	30.1	7.252×10^{-3}	B	8739.43
39.92	0.02321	100.2	5.648	30.15	7.428×10^{-3}	C	330691
60.18	0.1917	99.94	5.833	40.7	0.02461		
60.03	0.1734	for small saturator		60.01	0.1826		
60.06	0.1858	19.85	0.002224	79.96	1.130		
60.06	0.1779	19.90	0.002160	79.92	1.112		
60.16	0.1842	30.11	0.007276	100.09	5.798		
79.98	1.104	30.13	0.007481				
79.96	1.099	60.27	0.1996				

Di-*n*-butyl phthalate: vapor pressure vs. 1/T
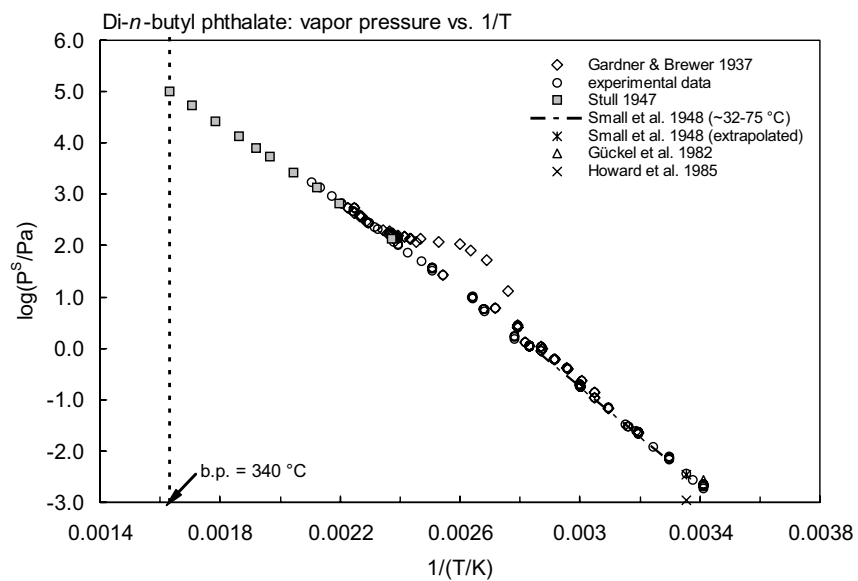
FIGURE 15.1.3.6.2 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-butyl phthalate.

15.1.3.7   Di-isobutyl phthalate (DIBP)
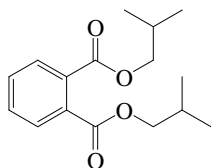
Common Name: Di-isobutyl phthalate
Synonym: DIBP
Chemical Name: phthalic acid diisobutyl ester, bis(2-methylpropyl)ester, 1,2-benzenedicarboxylic acid
CAS Registry No: 84-69-5
Molecular Formula: $C_{16}H_{22}O_4$
Molecular Weight: 278.344
Melting Point (°C):
    −58   (Staples et al. 1997)
Boiling Point (°C):
    296.5   (Lide 2003)
Density (g/cm³ at 20°C):
    1.040   (Fishbein & Albro 1972)
    1.049   (15°C, Weast 1982–83)
Molar Volume (cm³/mol):
    347.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    100   (Fishbein & Albro 1972)
    6.20   (shake flask-nephelometry, Hollifield 1979)
    20.3   (Leyder & Boulanger 1983)
    20.0; 5.1, 9.6   (recommended; calculated-QSAR, Staples et al. 1997)
    21.6   (calculated-UNIFAC, Thomsen et al. 1999)
    9.90   (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
    2.4×10^{-4}, 0.0773   (calculated-QSAR, Staples et al. 1997)
    0.00473   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa m³/mol at 25°C):
    0.0185   (recommended, Staples et al. 1997)
    0.133   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    4.11   (shake flask, Leyder & Boulanger 1983)
    4.43   (calculated-QSAR, Matthiessen et al. 1992)
    4.11   (quoted and recommended, Sangster 1993)
    4.11   (recommended, Hansch et al. 1995)
    4.11; 4.31, 4.46   (recommended; calculated-QSAR, Staples et al. 1997)
    4.46   (calculated-UNIFAC, Thomsen et al. 1999)
    4.27   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:
    3.10   (calculated-QSAR, fish, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

  3.14   (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
  3.01   (suspended solids, Staples et al. 1997)

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

  Volatilization:
  Photolysis:
  Oxidation: atmospheric photooxidation $t_{1/2}$ = 0.6–6.0 d (calculated, Staples et al. 1997)
      k_{OH} = 9.280 × 10^{-12} cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.89 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003).
  Hydrolysis:
      k(second-order alkaline) = (1.4 – 0.2) × 10^{-3} M^{-1} s^{-1} at 30°C in water (Wolfe et al. 1980b)
  Biodegradation: degradation $t_{1/2}$ = 3.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
      Aerobic biodegradation in aquatic environments, first order k = 0.8 d^{-1} with $t_{1/2}$ = 0.87 d in river water (Peterson & Staples 2003)
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
      k_2 = 0.134 d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)
      k_2 = 0.0114 d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

  Air: atmospheric photooxidation half-life of 0.6–6.0 d (calculated, Staples et al. 1997).
      photodegradation $t_{1/2}$ = 0.89 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)
  Surface water: biodegradation $t_{1/2}$ = 0.87 d in river water (Peterson & Staples 2003)
  Groundwater:
  Sediment:
  Soil: degradation $t_{1/2}$ = 3.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
  Biota:

15.1.3.8   Dipentyl phthalate (DPP)
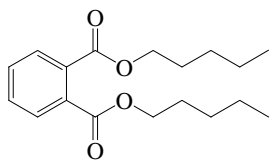
Common Name: Dipentyl phthalate
Synonym: DPeP, di-*n*-amyl phthalate
Chemical Name: dipentyl phthalate, phthalic acid diphenyl ester, 1,2-benzenedicarboxylic acid diphenyl ester
CAS Registry No: 131-18-0
Molecular Formula: $C_{18}H_{26}O_4$
Molecular Weight: 306.397
Melting Point (°C):
     < –54.5   (Stephenson & Malanowski 1987)
Boiling Point (°C):
     342   (Stephenson & Malanowski 1987)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
     299.8   (16°C, Stephenson & Malanowski 1987)
     391.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     99.16   (Small et al. 1948)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
     0.082   (shake flask-nephelometry, Hollifield 1979)
     0.1–0.8   (shake flask-GC, Leyder & Boulanger 1983)
     0.522, 1.69 (quoted, calculated-UNIFAC, Thomsen et al. 1999)
     1.30   calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
     5.68×10^{-4} (effusion method, extrapolated-Antoine eq., Small et al. 1948)
     log (P/mmHg) = 12.04 – 5191/(T/K); temp range 55–102°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine
        eq., effusion, data presented in graph, Small et al. 1948) (See figure at the end of this section.)
     0.0014   (20°C, extrapolated, tensimeter, measured range 63–111°C, Perry & Weber 1949)
     log (P/µmHg) = 13.57 – 4560/(T/K); temp range 63–111°C (pendulum-tensimeter method, Perry & Weber
        1949)
     5.68×10^{-4} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
     log (P_L/kPa) = 11.165 – 5191/(T/K); temp range 303–500 K (Antoine eq., liquid, Stephenson & Malanowski
        1987)
     0.00128   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C):
     0.302   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
     4.85   (shake flask, Leyder & Boulanger 1983; quoted, Sangster 1993, Hansch et al. 1995)
     5.33   (calculated-UNIFAC, Thomsen et al. 1999)
     5.12, 5.62   (calculated-QSPR, quoted lit., Cousins & Mackay 2000)

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

  9.03   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
  Volatilization:
  Photolysis:
  Oxidation:
  Hydrolysis:
  Biodegradation: degradation $t_{1/2}$ = 9.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);
    rate constant k = (9.12 ± 1.51) × 10^{-2} min^{-1} was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).
    aerobic biodegradation in aquatic environments, first order k = 1.3 d^{-1} with $t_{1/2}$ = 5.3 d in river water (Peterson & Staples 2003)
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
  Air:
 Surface water: biodegradation $t_{1/2}$ = 5.3 d in aerobic aquatic environments (Peterson & Staples 2003)
  Groundwater:
  Sediment:
  Soil: degradation $t_{1/2}$ = 9.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
  Biota:
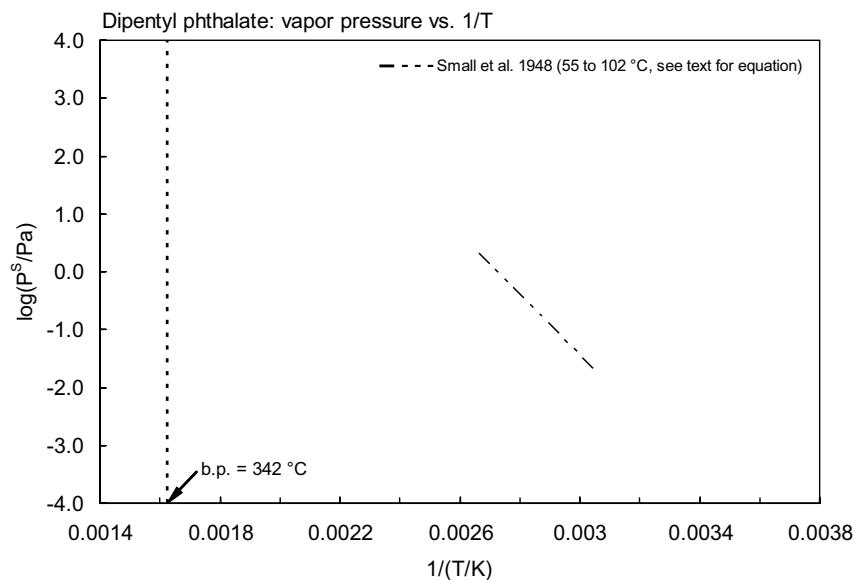
FIGURE 15.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for dipentyl phthalate.

15.1.3.9   Di-*n*-hexyl phthalate (DHP)
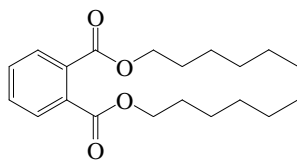
Common Name: Di-*n*-hexyl phthalate
Synonym: DHP, DnH(6)P
Chemical Name: Di-*n*-hexyl phthalate, dihexyl ester, 1,2-benzenedicarboxylic acid
CAS Registry No: 84-75-3, 68515-50-4
Molecular Formula: $C_{20}H_{30}O_4$, $C_6H_4[COOCH_2(CH_2)_4CH_3]_2$
Molecular Weight: 334.450
Melting Point (°C):
    –27.4   (Staples et al. 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C):
    0.990   (Fishbein & Abro 1972)
Molar Volume (cm³/mol):
    227.8   (20°C, calculated-density)
    436.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    102.9   (Small et al. 1948)
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):
    insoluble   (Fishbein & Abro 1972)
    0.24   (shake flask-HPLC/UV, Howard et al. 1985)
    0.05; 0.19, 0.049   (recommended; calculated-QSAR, Staples et al. 1997)
    0.046   (shake flask-GC, Ellington 1999)
    0.47   (calculated-UNIFAC method, Thomsen et al. 1999)
    0.159   (calculated-QSPR, Cousins & Mackay 2000)
    0.94, 0.52, 0.38   (10, 25, 35°C, shake flask-surface tension measurement, Thomsen et al. 2001) (See figure
                   at the end of this section.)
    0.070   (20°C, shake flask-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    $\log (P/mmHg) = 11.98 – 5381/(T/K)$; temp range 72–112°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine
        eq., effusion method, data presented in graph, Small et al. 1948) (See figure at the end of this section.)
    667   (at 210°C, Fishbein & Abro 1972)
    1.03×10^{-3} (Antoine eq., interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = –1.01167 – 1483.636/(T/K)$; temp range 288–303 K (Antoine eq.-I, Stephenson & Malanowski
        1987)
    $\log (P_L/kPa) = 11.105 – 5382/(T/K)$; temp range 343–387 K (Antoine eq.-II, liquid, Stephenson &
        Malanowski 1987)
    $\log (P_L/kPa) = –9.785 – 4805/(T/K)$; temp range 453–533 K (Antoine eq.-III for liquid, Stephenson & Malanowski
        1987)
    1.90×10^{-3} (gas saturation-GC, Howard et al. 1985)
    0.267   (quoted, Giam et al. 1994)
    0.67; 2.53×10^{-6}, 1.6×10^{-3} (recommended; calculated-QSAR, Staples et al. 1997)
    0.000345   (calculated-QSPR, Cousins & Mackay 2000)

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

    4.46   (recommended, Staples et al. 1997)

    0.726   (calculated-QSPR, Cousins & Mackay 2000)

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

    5.65–5.91   (HPLC-RT correlation, Howard et al. 1985)

    5.80   (quoted value of Howard et al. 1985, Sangster 1993)

    5.80   (Hansch et al. 1995)

    6.30; 6.57, 6.67   (recommended; calculated-QSAR, Staples et al. 1997)

    6.20   (calculated-UNFAC, Thomsen et al. 1999)

    6.00   (calculated-QSPR, Cousins & Mackay 2000)

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

    9.53   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

    4.72   (soil/sediment, Staples et al. 1997)

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

    Volatilization:

    Photolysis:

    Oxidation: atmospheric photooxidation $t_{1/2}$ = 0.4–4.0 d (calculated, Staples et al. 1997).

        k_{OH} = 14.929 × 10^{-12} cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.55 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

    Hydrolysis:

        Biodegradation: rate constant k = (6.86 ± 0.23) × 10^{-2} min^{-1} was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979);

        primary biodegradation rate constant k = 0.241 d^{-1} and $t_{1/2}$ = 2.93 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

    Biotransformation:

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

Half-Lives in the Environment:

    Air: atmospheric photooxidation $t_{1/2}$ = 0.4–4.0 d (calculated, Staples et al. 1997).

        Photodegradation $t_{1/2}$ = 0.55 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

        Surface water: primary biodegradation rate constant k = 0.241 d^{-1} and $t_{1/2}$ = 2.93 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).
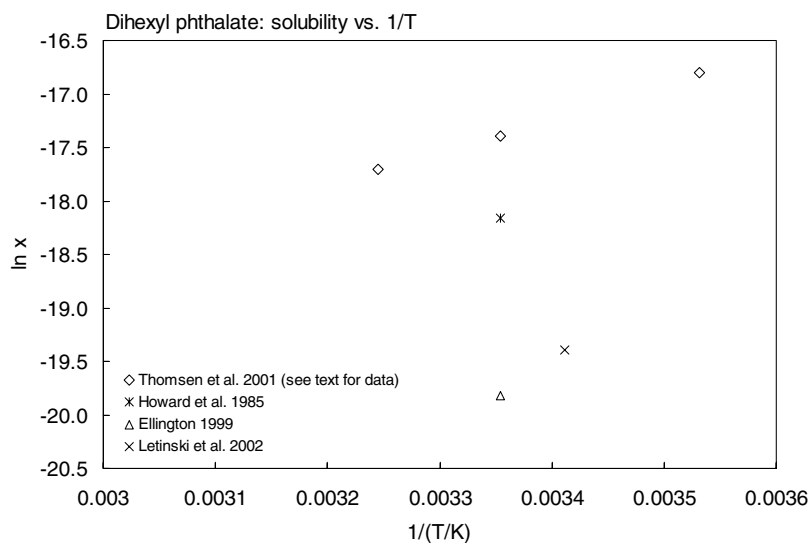
FIGURE 15.1.3.9.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for dihexyl phthalate.
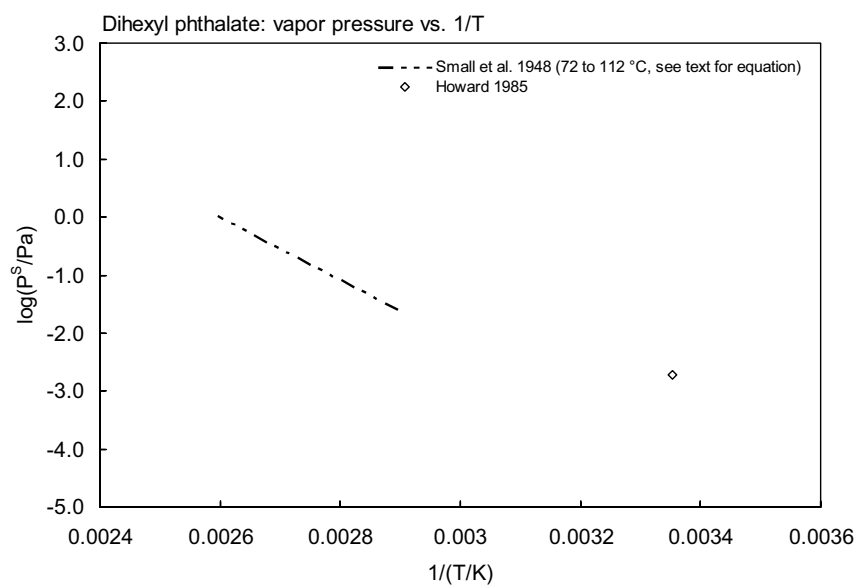
FIGURE 15.1.3.9.2 Logarithm of vapor pressure versus reciprocal temperature for dihexyl phthalate.

15.1.3.10 Butyl-2-ethylhexyl phthalate (BOP)
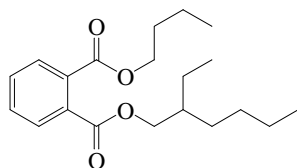
Common Name: Butyl-2-ethylhexyl phthalate
Synonym: BEHP, BOP
Chemical Name: Butyl-2-ethylhexyl phthalate
CAS Registry No: 85-69-8
Molecular Formula: $C_{20}H_{30}O_4$, $(C_4H_9OOC)C_6H_4(COOCH_2CH(C_2H_5)(CH_2)_3CH_3)$
Molecular Weight: 333.450
Melting Point (°C):
     −37   (Staples et al. 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
     446.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
     < 1.0   (shake flask-HPLC/UV spec., Howard et al. 1985)
     0.11; 0.02   (recommended; calculated-QSAR, Staples et al. 1997)
     0.075   (calculated-UNIFAC, Thomsen et al. 1999)
     0.385   (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
     1.47×10^{-5}; 3.2×10^{-3}, 0.016 (recommended; calculated-QSAR, Staples et al. 1997)
     5.37×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
     0.0405   (recommended, Staples et al. 1997)
     0.466   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
     5.93   (av. from OECD, Howard et al. 1985)
     3.70–7.88   (calculated-HPLC-RT, Howard et al. 1985)
     6.28; 6.5   (recommended, calculated-QSAR, Staples et al. 1997)
     6.20   (calculated-UNIFAC, Thomsen & Carlsen 1998)
     5.64   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
     9.37   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
     6.30   (suspended solids, Staples et al. 1997)

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

　　Volatilization:

　　Photolysis: direct photolysis rate $k_P = 2 \times 10^{-4}$ h^{-1} (EXAMS model, Wolfe et al. 1980a)

　　Oxidation: atmospheric photooxidation $t_{1/2} = 0.4–4.0$ d (calculated, Staples et al. 1997).

　　Hydrolysis:

　　　　k(second-order alkaline) $= (1.1 \pm 0.1) \times 10^{-4}$ M^{-1} s^{-1} for pH 10–12 at 30°C, with $t_{1/2}$(calc) = 2000 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)

　　　　k(acid catalyzed) $= 0.04$ M^{-1} h^{-1}, k(second order alkaline) $= 0.4$ M^{-1} h^{-1} in an aquatic environment (Wolfe et al. 1980a)

　　　　k(second-order alkaline) $= (1.1 \pm 0.1) \times 10^{-4}$ M^{-1} s^{-1} at 30°C in water with $t_{1/2} = 100–2000$ yr (Wolfe et al. 1980b)

　　Biodegradation: primary biodegradation rate constant $k = 0.153$ d^{-1} and $t_{1/2} = 4.55$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984)

　　Biotransformation:

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

Half-Lives in the Environment:

　　Air: atmospheric photooxidation $t_{1/2} = 0.4–4.0$ d (calculated, Staples et al. 1997).

　　Surface water: hydrolysis $t_{1/2} = 100–2000$ yr (Wolfe et al. 1980b; Callahan et al. 1979);

　　　　primary biodegradation rate constant $k = 0.153$ d^{-1} and $t_{1/2} = 4.55$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

　　Groundwater:

　　Sediment:

　　Soil:

　　Biota:

15.1.3.11 Di-*n*-octyl phthalate (DOP)
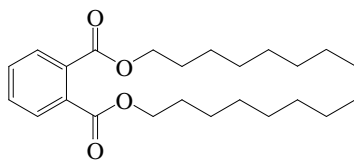
Common Name: Di-*n*-octyl phthalate
Synonym: di-*n*-octyl phthalate, DOP, *o*-benzenedicarboxylic acid dioctyl ester, *n*-dioctyl phthalate, octyl phthalate, dioctyl-*o*-benzenedicarboxylate
Chemical Name: di-*n*-octyl phthalate
CAS Registry No: 117-84-0
Common Molecular Formula: $C_{24}H_{38}O_4$, $C_6H_4(COOC_8H_{17})_2$
Molecular Weight: 390.557
Melting Point (°C):
    −25.0   (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982; Lide 2003)
Boiling Point (°C):
    220.0   (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982)
Density (g/cm^3 at 20°C):
    0.978   (Fishbein & Albro 1972; Ellington 1999)
Molar Volume (cm^3/mol):
    399.3   (20°C, calculated-density)
    524.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    50.0   (20°C, Fishbein & Albro 1972)
    3.0   (shake flask-GC, Wolfe et al. 1979)
    3.0   (shake flask-GC, Wolfe et al. 1980a,b)
    0.285   (24°C, tech. grade, Verschueren 1983)
    0.022   (generator column-HPLC/UV, DeFoe et al. 1990)
    0.020, 0.040   (synthesized phthalates by turbidity inflection-HPLC/UV, DeFoe et al. 1990)
    1.96   (calculated-molar volume, Wang et al. 1992)
    0.0005   (recommended, Staples et al. 1997)
    0.00051; 0.00049   (shake flask: slow stirring; no-stirring, GC/FID, Ellington 1999)
    0.0092   (calculated-UNIFAC method, Thomsen et al. 1999)
    0.0249   (calculated-QSPR, Cousins & Mackay 2000)
    0.00040   (20°C, shake flask-GC/MS, Letinski et al. 2002)
    0.00040, 0.00042 (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    4.21×10^{-6} (20°C, tensimeter, extrapolated, measured range 113–162°C, Perry & Weber 1949)
    log (P/µmHg) = 14.68 −5620/(T/K); temp range 113–162°C (tensimeter, Perry & Weber 1949)
    0.0187   (estimated by analogy to Henry's law constant, Mabey et al. 1982)
    2.92×10^{-5} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
    log (P$_L$/kPa) = 9.897 − 5197.4/(T/K), temp range: 423–523 K, (Antoine eq., Stephenson & Malanowski 1987)
    1.33×10^{-5} (recommended, Staples et al. 1997)
    2.52×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa m^3/mol at 25°C):
    0.557   (calculated-P/C, Wolfe et al. 1980a)
    1.722   (calculated-P/C, Mabey et al. 1982)
    0.0297   (quoted from WERL Treatability Data, Ryan et al. 1988)

    10.435   (selected, Staples et al. 1997)
    0.0249   (calculated-QSPR, Cousins & Mackay 2000)

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

    9.2   (calculated as per Leo et al. 1971, Callahan et al. 1979)
    9.2   (calculated, Wolfe et al. 1979)
    8.06   (HPLC-RT correlation; McDuffie 1981)
    8.92   (calculated-CLOGP for synthesized phthalate, DeFoe et al. 1990)
    5.22   (shake flask, log P database, Hansch & Leo 1987)
    8.06   (recommended, Staples et al. 1997)
    6.99   (calculated-UNIFAC method, Thomsen et al. 1999)
    7.73   (calculated-QSPR, Cousins & Mackay 2000)

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

    10.53   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

    2.82, 3.97, 0.064, 3.72, 2.64 (in lab. model ecosystem after 3 d: alga, daphnia, mosquito fish, mosquito larvae,
        snails, Sanborn et al. 1975)
    4.45, 3.41, 3.97, 3.97, 4.13   (in lab. model ecosystem after 33 d: alga, daphnia, mosquito fish, mosquito larvae,
        snails, Sanborn et al. 1975)
    3.46   (bacteria, calculated-K_{OW}, Wolfe et al. 1980a)
    8.59   (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

    4.28   (calculated, Wolfe et al. 1980a)
    9.56   (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
    7.91   (sediment, calculated-K_{OW}, Pavlou & Weston 1983, 1984)
    7.60   (calculated-K_{OW}, Kollig 1993)
    6.30   (suspended solids, calculated-K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)

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

    Volatilization:
    Photolysis: direct photolysis rate $k_P = 2 \times 10^{-4}$ h^{-1} (EXAMS model, Wolfe et al. 1980a)
    Oxidation: k = 18 M s^{-1}, free radical oxidation rate constant in an aquatic environment (Wolfe et al. 1980a)
        k << 360 M^{-1} h^{-1} for singlet oxygen and k = 1.4 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)
        photooxidation $t_{1/2}$ = 4.5–44.8 h in air, based on estimated rate constant for the vapor phase reaction with
            hydroxyl radical in air (Howard et al. 1991)
        photooxidation $t_{1/2}$ = 0.3–3.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)
        $k_{OH} = 20.581 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.40 d based on a global, seasonal and diurnal average
            OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)
    Hydrolysis:
        phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2}$ = 4 months to 100 yr at pH 8 and 30°C
            (Wolfe et al. 1980a)
        k(acid catalyzed) = 0.04 M^{-1} h^{-1}, k(second order alkaline) = 59 M^{-1} h^{-1} in an aquatic environment (Wolfe
            et al. 1980a)
        k(base) = 7.4 M^{-1} h^{-1} at pH 7 and 25°C (Ellington et al. 1987)
        $t_{1/2}$ = 107 yr at pH 7, $t_{1/2}$ = 1 yr at pH 9 and 25°C (Howard et al. 1991; selected, Staples et al. 1997).
    Biodegradation: the pseudo first-order degradation rate constant k = 0.14 d^{-1} corresponding to $t_{1/2}$ = 5 d in a
        model ecosystem (Sanborn et al. 1975);
        degradation $t_{1/2}$ = 8 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
        rate constant k ~ $(1.57 \pm 0.17) \times 10^2$ min^{-1} from retention times of reverse phase chromatography (estimated,
            Urushigawa & Yonezawa 1979);
        microbial degradation rate constant k = 2×10^{-4} h^{-1} in an aquatic environment (Wolfe et al. 1980a)

significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate $k < 0.5$ d^{-1} (Tabak et al. 1981; quoted, Mills et al. 1982);

biodegradation rate constant $k = 7.4 \times 10^{-9}$ $mL \cdot cell^{-1} \cdot d^{-1}$ at 30°C in water (Scow 1982);

aqueous aerobic $t_{1/2} = 168–672$ h, based on unacclimated and acclimated aqueous screening test data; aqueous anaerobic $t_{1/2} = 4320–8760$ h, based on acclimated anaerobic screening test data (Howard et al. 1991);

rate constant $k = 0.0014$ h^{-1} with $t_{1/2} = 513.4$ h for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.7$ d^{-1} with $t_{1/2} = 1.0$ d in river water (Peterson & Staples 2003)

anaerobic biodegradation, first order rate $k = 0.006–0.0336$ d^{-1} with $t_{1/2} = 115–20.6$ d in undiluted digester sludge of different DOP concn, batch incubation (Peterson & Staples 2003)

Biotransformation: $k = 3.1 \times 10^{-10}$ $mL \cdot cell^{-1} \cdot h^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a);

microbial transformation $k = (3.7 \pm 0.6) \times 10^{-13}$ $L \cdot organism^{-1} \cdot h^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

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

$k_2 = 3.69 \times 10^{-5}$ d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6}$ d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.5–44.8$ h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.40$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: degradation $t_{1/2} = 5$ d in an aquatic model ecosystem (Sanborn et al. 1975);

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

biodegradation $t_{1/2} = 1.0$ d in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 336–8760$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} = 8$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2} = 10–50$ d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

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

Biota:

15.1.3.12 Di-isooctyl phthalate (DIOP)
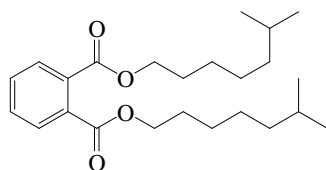
Common Name: Di-isooctyl phthalate
Synonym: DIOP
Chemical Name:
CAS Registry No: 27554-26-3
Molecular Formula: $C_{24}H_{38}O_4$
Molecular Weight: 390.557
Melting Point (°C):
    –4   (Fishbein & Albro 1972)
    –46   (Staples et al. 1997)
Boiling Point (°C):
    270   (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
    524.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.09   (shake flask-GC, Howard et al. 1985)
    0.001; 0.00024, 0.00081   (recommended; calculated-QSAR, Staples et al. 1997)
    2.49×10^{-3} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    1.55×10^{-4} (dew-point and tensimeter methods, extrapolated from Clausius-Clapeyron eq., Werner 1952)
    log (P/micron) = $- 4829/(T/K) + 13.262$; temp range 70–210°C, (exptl. data fitted to the Clausius-Clapeyron eq., Werner 1952)
    7.4×10^{-4} (gas saturation method, Howard et al. 1985)
    log (P/mmHg) = $24.8803 - 5.5821 \times 10^3/(T/K) - 1.2116 \cdot \log (T/K) - 1.547 \times 10^{-2} \cdot (T/K) + 6.5101 \times 10^{-6} \cdot (T/K)^2$; temp range 260–851 K (vapor pressure eq., Yaw et al. 1994)
    1.55×10^{-4}, 7.4×10^{-4}, 4.53×10^{-5} (quoted, Staples et al. 1997)
    7.5×10^{-4}; 1.33×10^{-4}, 2.67×10^{-8}, 1.87×10^{-4} (recommended; calculated-QSAR, Staples 1997)
    2.52×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    3.95   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    8.0; 8.39   (recommended; calculated-QSAR, Staples et al. 1997)
    7.73   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    10.53   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

    Volatilization:
    Photolysis:
    Oxidation: atmospheric photooxidation $t_{1/2}$ ~ 0.3–3.0 d (Estimated, Staples et al. 1997).
    Hydrolysis: aqueous hydrolysis $t_{1/2}$ ~ 157 yr (estimated, Staples et al. 1997).
    Biodegradation: primary biodegradation rate constant k = 0.082 d^{-1} and $t_{1/2}$ = 8.82 d in an acclimated shake flask
        CO_2 evolution test (Sugatt et al. 1984).
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

    Air: atmospheric photooxidation $t_{1/2}$ ~ 0.3–3.0 d (estimated, Staples et al. 1997).
    Surface water: primary biodegradation rate constant k = 0.082 d^{-1} and $t_{1/2}$ = 8.82 d in an acclimated shake flask
        CO_2 evolution test (Sugatt et al. 1984);
        aqueous hydrolysis $t_{1/2}$ ~ 157 yr (estimated, Staples et al. 1997).
    Groundwater:
    Sediment:
    Soil:
    Biota:

15.1.3.13 *bis*-(2-Ethylhexyl) phthalate (DEHP)
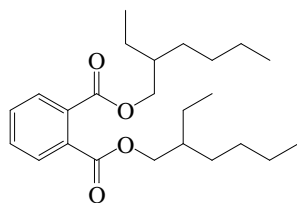
Common Name: Di-(2-ethylhexyl) phthalate
Synonym: DEHP, bis(2-ethylhexyl) phthalate, di-(2-ethylhexyl)orthophthalate, bis(2-ethylhexyl) phthalic acid ester, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate, 1,2-benzenedicarboxylic acid bis(2-ethylhexyl) ester
Chemical Name: bis(2-ethylhexyl) phthalate, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate
CAS Registry No: 117-81-7
Molecular Formula: $C_{24}H_{38}O_4$, o-$C_6H_4(COOCH_2CH(C_2H_5)C_4H_9)_2$
Molecular Weight: 390.557
Melting Point (°C):
    –55.0   (Verschueren 1983; Lide 2003)
Boiling Point (°C):
    384.0   (Dean 1985; Riddick et al. 1986; Lide 2003)
Density (g/cm³ at 20°C):
    0.9850   (Fishbein & Albro 1972)
    0.9843   (Riddick et al. 1986)
Molar Volume (cm³/mol):
    396.1   (20°C, calculated-density, Stephenson & Malanowski 1987)
    524.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    107.1, 105.9 (Small et al. 1948)
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):
    100   (20°C, Fishbein & Albro 1972)
    50.0   (from Monsanto Chemical Co. data sheets, Peakall 1975)
    0.60   (Branson 1978; Kenaga & Goring 1980)
    0.285   (shake flask-nephelometry on technical grade DEHP, Hollifield 1979)
    100   (quoted from Metcalf & Lu 1973, Hollifield 1979; Garten & Trabalka 1983)
    2.49   (Neely 1979; quoted, Neely & Blau 1985; Lyman 1985; Elzerman & Coates 1987)
    0.40   (shake flask-GC, Wolfe et al. 1979, 1980a, b)
    1.16   (solubility in 35 L instant ocean solution, Giam et al. 1980)
    0.047   (from OECD 1979/80, Klöpffer et al. 1982)
    0.041   (20°C, shake flask-UV, Leyder & Boulanger 1983)
    0.34 ± 0.04   (shake flask-HPLC/UV, Howard et al. 1985)
    < 100   (quoted, Riddick et al. 1986)
    0.27; 0.36   (centrifugation method, turbidity inflection method, DeFoe et al. 1990)
    9.8×10^{-6} to 0.633 (lit. values, Sabljic et al. 1990)
    0.003   (recommended, Staples et al. 1997)
    0.0249   (calculated-QSPR, Cousins & Mackay 2000)
    0.017   (22°C, shake flask-surface tension measurement, Thomsen et al. 2001)
    0.0019   (20°C, shake flask-GC/MSD, Letinski et al. 2002)
    0.00285, 0.00024   (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

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

1.45×10^{-5} (20°C, extrapolated, tensimeter, measured range 95–145°C, Hickman et al. 1937)

$\log (P/\mu Hg) = 15.116 – 5590/(T/K)$; temp range 95–145°C (Hickman et al. 1937)

1.93×10^{-5} (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log (P/mmHg) = 12.12 – 5590/(T/K)$ (Antoine eq., quoted from Barclay & Butler 1938; Small et al. 1948)

$\log (P/mmHg) = 12.47 – 5757/(T/K)$; pressure range 5×10^{-2} to 10^{-4} mmHg (effusion, data presented in graph and Antoine eq., Small et al. 1948)

1.51×10^{-5} (20°C, extrapolated, tensimeter, measured range 99–148°C, Perry & Weber 1949)

$\log (P/\mu Hg) = 14.62 – 5440/(T/K)$; temp range 99–148°C (pendulum tensimeter method, Perry & Weber 1949)

8.26×10^{-6}* (measured by dew-point and tensimeter methods, temp range 120–225°C, extrapolated from Antoine eq., Werner 1952)

$\log (P/micron) = 12.639 – 3811/(201.2 + t/°C)$; temp range 120–225°C (Antoine eq., Dew-Point and Tensimeter methods, data presented in graph, Werner 1952)

2.70×10^{-5} (20°C, calculated-Antoine eq., Weast 1972–73)

1.73×10^{-5} (submicron droplet evaporation, Chang & Davis 1976)

5.81×10^{-5} (36°C, submicron droplet evaporation, Davis & Ray 1977)

5.84×10^{-6} (17°C, submicron droplet evaporation, measured range 17–31°C, Ray et al. 1979)

$\log (P/mmHg) = 12.729 – 5822/(T/K)$; temp range 17–31°C (submicron droplet evaporation, Ray et al. 1979)

6.0×10^{-6}*, 1.30×10^{-5} (20°C, effusion-vapor pressure balance, gas saturation method, OECD 1981)

$\log (P/mmHg) = 10.086 – 5010.357/(T/K)$; temp range 10–50°C (Antoine eq., gas saturation, OECD 1981)

$\log (P/mmHg) = 13.243 – 6035.017/(T/K)$; temp range 80–120°C (Antoine eq., effusion, OCED 1981)

5.50×10^{-6} (20°C, estimated-evaporation rate, Dobbs & Cull 1982)

7.01×10^{-8} (20°C, gas saturation, measured range 120–140°C, Potin-Gauthier et al. 1982)

$\log (P/mmHg) = 18.408 – 8112.265/(T/K)$; temp range 120–140°C (Potin-Gauthier et al. 1982)

0.00293, 1.87×10^{-6}, 7.47×10^{-4} (estimation-structure based methods, Tucker et al. 1983)

$8.6 \pm 6.6) \times 10^{-4}$ (gas saturation-HPLC/UV, Howard et al. 1985)

70, 700 (literature values, Riddick et al. 1986)

5.08×10^{-5} (extrapolation-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 11.8564 – 6416.2/(36.74 + T/K)$; temp range 373–660 K (Antoine eq., Stephenson & Malanowski 1987)

$(1.20–2.40) \times 10^{-5}$ (quoted from OECD interlaboratory studies, Hinckley et al. 1990)

1.90×10^{-5} (GC-RT correlation, Hinckley et al. 1990)

1.2×10^{-4}* (40°C, OECD Vapour Pressure Curve Guideline 104, temp range 40–80°C, OECD 1993)

$\log (P/mmHg) = –0.7422 – 7.2012 \times 10^{3}/(T/K) + 9.9887 \cdot \log(T/K) – 2.2697 \times 10^{-2} \cdot (T/K) + 8.2181 \times 10^{-6} \cdot (T/K)^2$; temp range 350–886 K (vapor pressure eq., Yaw et al. 1994)

1.50×10^{-4}* (40°C, Knudsen effusion with different orifice diameters and variable cell height, measured range 40–80°C, Goodman 1997)

$\log (P/Pa) = 14.90 – 5911/(T/K)$; temp range 40–80°C (Knudsen effusion, Goodman 1997)

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

0.0446 (calculated-P/C, Wolfe et al. 1980a)

1.1140 (calculated, Lyman et al. 1982)

0.0304 (20–25°C, calculated-P/C, Mabey et al. 1982)

0.0263, 3.14 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)

0.0042 (estimated-P/C, Lyman 1985)

0.101 (estimated as per Hine & Mookerjee 1975, Lyman 1985)

0.0041 (calculated-P/C, Mackay 1985, Neely & Blau 1985)

0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)

1.4940 (calculated-P/C, Meylan & Howard 1991)

1.1970 (estimated-bond contribution, Meylan & Howard 1991)

1.7324 (selected, Staples et al. 1997)

3.95 (calculated-QSPR, Cousins & Mackay 2000)

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

3.58	(Lu & Metcalf 1975)
4.20	(Mayer 1976)
5.30	(Hirzy et al. 1978)
8.73	(calculated, Wolfe et al. 1979)
5.11, 4.66–5.45	(shake flask method: mean, range, OECD 1981)
7.86	(HPLC-extrapolated from alkylbenzenes, Harnish et al. 1983)
5.03	(shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
9.64	(quoted lit. calculated value, Leyder & Boulanger 1983)
7.94	(HPLC-RT correlation, Howard et al. 1985)
7.80, 8.90	(HPLC-RT correlation, TLC-RT, Klein et al. 1988)
7.453 ± 0.061	(slow-stirring-GC, De Bruijn et al. 1989)
5.22	(shake flask method, Brooke et al. 1990)
7.86, 9.68	(HPLC method, calculated, Brooke et al. 1990)
7.137 ± 0.153	(stir-flask method by BRE, Brooke et al. 1990)
7.453 ± 0.061	(stir-flask method by RITOX, Brooke et al. 1990)
7.88	(recommended, Sangster 1993)

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

10.53	(calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

2.11	(fish, Metcalf et al. 1973)
5.03	(mosquito larvae, Metcalf et al. 1973)
4.13, 3.49, 3.72, 3.36, 2.36	(scud, midge larvae, waterflea, mayfly, sowbug, Sanders et al. 1973)
3.56, 2.54, 2.62, 2.76, 2.66	(scud, midge, waterflea, mayfly, fathead minnow, 14-d exposure, Mayer & Sanders 1973)
3.14	(fathead minnow, 28-d exposure, Mayer & Sanders 1973)
2.76	(fathead minnow, 56-d exposure, Mayer 1976)
2.93	(fathead minnow, Veith et al. 1979)
2.90, 2.15	(fathead minnow, Branson 1978)
2.06	(bluegill sunfish, Barrows et al. 1980)
–1.92	(adipose tissue of female Albino rats, Geyer et al. 1980)
3.95	(bacteria, calculated-K_{OW}, Wolfe et al. 1980a)
0.84–1.05, 1.01–1.22, 1.03–1.13	(oyster, shrimp, fish, Wofford et al. 1981)
1.04	(oyster, Wofford et al. 1981; quoted, Zaroogian et al. 1985)
2.93, 2.88	(fish: quoted, calculated-K_{OW}, Mackay 1982)
2.32	(*Daphnia maga*, Brown & Thompson 1982a)
3.37, 3.42, 3.40	(mussel *Mytilus edulis*, Brown & Thompson 1982b)
8.36	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.49, 2.11	(fish: flowing water, microcosm conditions, Graten & Trabalka 1983)
3.73, 3.57	(alga *Chlorella*, calculated-K_{OW}, Geyer et al. 1984)
2.80	(sheephead minnows, predicted-pharmacokinetic model, Karara & Hayton 1984)
2.66, 3.73, 3.48	(golden orfe, algae, activated sludge, Freitag et al. 1982)
1.60, 3.73, 3.48	(golden ide, algae, activated sludge, Freitag et al. 1985)
2.96, 2.87	(oyster, estimated values, Zaroogian et al. 1985)
2.96, 2.87	(sheephead minnows, estimated values, Zaroogian et al. 1985)
2.76	(quoted, Isnard & Lambert 1989)
0.204–1.71	(rainbow trout, BCF to decline as body wt. increased, Tarr et al. 1990)
2.94	(fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

4.0–5.0	(soil, calculated values, Kenaga 1980; Wolfe et al. 1980a)
4.756	(sediment-water, calculated-K_{OW} and S, Wolfe et al.1980a)
9.301	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)

4.31, 5.27, 4.90, 4.98 (estimated-K$_{OW}$, Karickhoff 1985)
4.24, 5.06 (estimated-S, Karickhoff 1985)
5.10 (best estimate, expected at low sediment concn. of < 10^{-4}/mL, Karickhoff 1985)
5.00 (soil/sediment, Neely & Blau 1985)
4.94 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986;)
5.22 (soil, calculated- MCI χ and fragment contribution, Meylan et al. 1992)
2.60 (activated carbon, calculated-MCI χ, Blum et al. 1994)
7.13 (calculated-K$_{OW}$, Kollig 1993)
4.34, 6.00 (suspended solids, calculated-K$_d$ assuming a 0.1 org. carbon fraction, Staples et al. 1997)

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

Volatilization: calculated evaporation rate k = 0.00052 cm/h corresponding to t$_{1/2}$ = 132600 h for a pond of 1 m deep (Branson 1978).

Photolysis: rate constant for direct photolysis k = 2 × 10^{-4} h^{-1} in natural water (Wolfe et al. 1980a);
t$_{1/2}$ ~ 143 d in water is estimated to be 143 d (Wolfe et al. 1980a; quoted, Howard 1989);
atmospheric t$_{1/2}$ = 3500–4800 h and aqueous t$_{1/2}$ = 3500–4800 h, based on measured rate of aqueous photolysis for DMP (Howard 1991).
Aqueous photolysis k = 0.9 h^{-1} and t$_{1/2}$ = 0.75 h (Jin et al. 1999, quoted, Peterson & Staples 2003)

Oxidation: the free radical oxidation rate constant k = 18 M·s^{-1} (Wolfe et al. 1980b);
photooxidation t$_{1/2}$ = 44–584 d in water, based on estimated rate constant for the reaction with hydroxyl radicals in water (Wolfe et al. 1980; quoted, Howard et al. 1991);
rate constant k << 360 M^{-1}·h^{-1} for singlet oxygen and k = 7.2 M^{-1}·h^{-1} for peroxy radical (Mabey et al. 1982);
photooxidation t$_{1/2}$ = 2.9–29 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
predicted atmospheric photooxidation t$_{1/2}$ = 0.2–2.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).
k$_{OH}$ = 21.955 × 10^{-12} cm^3 molecule^{-1} s^{-1} and t$_{1/2}$ = 0.38 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis: second order alkaline hydrolysis rate constant k = 1.1 × 10^{-4} M^{-1}·s^{-1} for pH 10–12 at 30°C in water (Wolfe et al. 1979, 1980b; quoted, Callahan et al. 1979);
t$_{1/2}$ = 100 to 2000 yr for hydrolytic degradation alone in the eutrophic lake ecosystem at steady-state increase (Wolfe et al. 1080a);
t$_{1/2}$(calc) = 2000 yr at pH 7 in water (calculated per Radding et al. 1977; quoted, Callahan et al. 1979; Howard 1989; Howard et al. 1991);
k(exptl.) = 9.5 × 10^{-7} d^{-1} at pH 7 and 25°C while estimated rate constant k = 1.46 × 10^{-6} d^{-1} at pH 7 and 30°C (Neely 1985);
first-order hydrolysis t$_{1/2}$ = 2000 yr at pH 7, based on measured base catalyzed hydrolysis rate constant (Howard et al. 1991; selected, Staples et al. 1997).

Biodegradation: approximately calculated rate constant k = 0.091 d^{-1} in pond water plus sediment incubated under aerobic conditions based on time for 50% degradation (Johnson & Lulves 1975; quoted, Klečka 1985);
estimated biodegradation t$_{1/2}$ ~ 4–5 wk by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);
degradation t$_{1/2}$ = 1.3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);
rate constant k = 0.023 d^{-1} in river water incubated under aerobic conditions (Klečka 1985);
rate constant k(mineralization rate divided by initial substrate concn.) = 0.028 ± 0.013 d^{-1} in lake water incubated under aerobic conditions (Subba-Rao et al. 1982; quoted, Klečka 1985);
t$_{1/2}$ = 2.0–3.0 wk, based on river die-away test data (Hattori et al. 1975; Saeger & Tucker 1976; Wolfe et al. 1980; estimated, Howard 1989);
t$_{1/2}$ = 0.8 d in activated sludge (Saeger & Tucker 1976; estimated, Howard 1989);
microbial degradation rate constant k = 4.2 × 10^{-12} mL·organism^{-1}·s^{-1} (Wolfe et al. 1980a);
significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate k < 0.5 d^{-1} (Tabak et al. 1981; quoted, Mills et al. 1982);
aqueous aerobic t$_{1/2}$ = 120–550 h, based on grab sample die-away test data (Schouten et al. 1979 and Johnson & Lulves 1975; estimated, Howard 1991); aqueous anaerobic t$_{1/2}$ = 980–9336 h, based on anaerobic

die-away test data (Howard et al. 1991) and anaerobic aqueous screening studies (Horowitz et al. 1982 and Shelton et al. 1984; estimated, Howard et al. 1991);

mean rate constant $k = 0.136$ d^{-1} corresponding to $t_{1/2} = 5.25$ d in shake flask biodegradation experiment (Sugatt et al. 1984);

more than 90% of initial 3.3 mg/L will be degraded in activated sludge systems in 2–5 d (O'Grady et al. 1985);

greater than 50% loss in microbial degradation in less than 20 d under aerobic conditions, very low under anaerobic conditions in garden soil (Shanker et al. 1985);

readily metabolized in uninoculated Erie slit loam with the absence of nonaqueous-phase liquids (NAPLs) for about 20 d (Efroymson & Alexander 1994)

biphasic microbial mineralization kinetics: $k = 0.0044$ d^{-1} with $t_{1/2} = 158$ d at 5°C, $k = 0.0081$ d^{-1} with $t_{1/2} = 86$ d at 10°C, and $k = 0.0134$ d^{-1} with $t_{1/2} = 52$ d at 20°C in agriculture soil for phase I; and $t_{1/2} = 224$ d at 5°C, $t_{1/2} = 187$ d at 10°C and $t_{1/2} = 73$ d at 20°C in agriculture soil for phase II. Rate $k = 0.0023$ d^{-1} with $t_{1/2} = 301$ d at 5°C, $k = 0.0055$ d^{-1} with $t_{1/2} = 125$ d at 10°C, and $k = 0.0127$ d^{-1} with $t_{1/2} = 55$ d at 20°C in sludge-amended soil for phase I and $t_{1/2} \geq 365$ d at 5°C, $t_{1/2} = 337$ d at 10°C and $t_{1/2} = 150$ d at 20°C in sludge-amended soil for phase II kinetics in laboratory microcosms. At 20°C, aerobic mineralization rate $k = 0.0182$ d^{-1} with $t_{1/2} = 37$ d for phase I, $t_{1/2} = 51$ d for phase II in well-mixed sludge, $k = 0.0058$ d^{-1} with $t_{1/2} = 120$ d for phase I, $t_{1/2} \geq 365$ d for phase II in aggregate sludge, aerobic $k = 0.0127$ d^{-1} with $t_{1/2} = 55$ d for phase I, $t_{1/2} = 150$ d for phase II and anaerobic $k = 0.0023$ d^{-1} with $t_{1/2} = 301$ d for phase I, $t_{1/2} \geq 365$ d for phase II in sludge-amended soil (Madsen et al. 1999).

aerobic biodegradation in aquatic environments, first order $k = 0.023$ d^{-1} with $t_{1/2} = 30$ d in unstirred river water, $k = 0.2$ d^{-1} with $t_{1/2} = 3.5$ d in shaken river water, $k = 1.73$ d^{-1} with $t_{1/2} = 0.4$ d field data, estuarine sediment (Peterson & Staples 2003)

aerobic soil degradation, pseudo-first-order $k = 0.035$ d^{-1} with $t_{1/2} = 2.0$ d in loam; $k = 0.010$ d^{-1} with $t_{1/2} = 69.3$ d in sand; $k = 0.033$ d^{-1} with $t_{1/2} = 21$ d in outdoor lysimeter, loam; $k = 0.013$ d^{-1} with $t_{1/2} = 53.3$ d in outdoor lysimeter, sand; $k = 0.12$ d^{-1} with $t_{1/2} = 5.6$ d in garden soil; $k = 0.040$ d^{-1} with $t_{1/2} = 17.3$ d in soil with 2% OC-organic carbon; $k = 0.019$ d^{-1} with $t_{1/2} = 36.5$ d in soil with 3.3% OC; $k = 0.015$ d^{-1} with $t_{1/2} = 46.2$ d in soil with 1.6% OC and $k = 0.012$ d^{-1} with $t_{1/2} = 58$ d in sludge amended loam. For anaerobic degradation, first order rate $k > 0.3$ d^{-1} with $t_{1/2} < 2.3$ d in undiluted digester sludge, batch incubation; $k = 0.013$ d^{-1} with $t_{1/2} = 53.3$ d in flood soil;, $k = 0.69$ d^{-1} with $t_{1/2} = 1.0$ d field data, sediment (Peterson & Staples 2003)

Biotransformation: $k = 4.2 \times 10^{-12}$ mL·cell^{-1}·h^{-1} for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982);

microbial transformation $k = (4.2 \pm 0.7) \times 10^{-15}$ L·organism^{-1}·h^{-1} in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

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

$t_{1/2} = 7$ d for elimination of DEHP from fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2} = 6.2$ to 18.3 d with a mean value of 12.2 d after 56 d exposure period (fathead minnows, Mayer 1976);

$k_1 = 76$ mL g^{-1}·h^{-1} (fish, Branson 1978);

depuration $t_{1/2} = 72$ h (tissues of bluegill sunfish, Barrows et al. 1980).

$k_2 = 3.69 \times 10^{-5}$ d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6}$ d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} =$ half-life of 2.9–29 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991);

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

Photodegradation $t_{1/2} = 0.38$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} \sim 4$ to 5 wk in river water by naturally occurring, mixed microbial populations (Saeger & Tucker 1976);

$t_{1/2} = 5$ d in a model ecosystem (Verschueren 1983);

$t_{1/2} = 5.25$ d in an acclimated shake flask CO$_2$ evolution biodegradation experiment (Sugatt et al. 1984)

$t_{1/2} = 120$-550 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}$. = 0.3–30 d in estuarine river water with sediment and river water (Peterson & Staples 2003)

Ground water: $t_{1/2}$ = 240–9336 h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2}$ = 1.3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

biodegradation $t_{1/2}$ < 20 d under anaerobic conditions in a garden soil (Shanker et al. 1985);

$t_{1/2}$ = 10–50 d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

degradation $t_{1/2}$ = 39 d for initial phase, $t_{1/2}$ = 51 d for the late phase in sludge-amended quartz; $t_{1/2}$ = 58 d for initial phase and $t_{1/2}$ = 147 d for sludge-amended soil, $t_{1/2}$ = 58 d for initial phases and $t_{1/2}$ = 84 d in sludge slurry; $t_{1/2}$ = 9 d for initial phases, $t_{1/2}$ = 35 d for late phase in sludge-amended soil + strain SDE-2 (Roslev et al. 1998)

overall $t_{1/2}$ = 120–550 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

degradation by microorganism in biometer systems, $t_{1/2}$ = 66 d in silty sand standard metabolism experiments, $t_{1/2}$ = 102 d corrected standard conditions, $t_{1/2}$ = 170 d in simulated outdoor conditions; $t_{1/2}$ = 20 d in silty loam standard conditions, $t_{1/2}$ = 30 d corrected standard conditions, $t_{1/2}$ = 31 d in simulated outdoor conditions at constant soil moisture and 20°C; degradation by microorganism in outdoor experiments in small lysimeter systems: $t_{1/2}$ = 54 d outdoor fallow and $t_{1/2}$ = 200 d outdoor barley in silty sand, and $t_{1/2}$ = 21 d outdoor fallow, $t_{1/2}$ = 14 d outdoor barley in silty loam (Rüdel et al. 1993)

microbial mineralization $t_{1/2}$ = 158, 86 and 52 d at 5, 10, and 20°C, respectively, in soil; $t_{1/2}$ = 301, 125 and 55 d at 5, 10 and 20°C in sludge-amended soil in phase I degradation kinetics; $t_{1/2}$ = 224, 187 and 73 d at 5, 10, and 20°C, respectively, in soil; $t_{1/2}$ = 365, 337 and 150 d at 5, 10 and 20°C in sludge-amended soil in phase II degradation kinetics. At 20°C, $t_{1/2}$ varies between 77–89 d and 100–127 d for phase I and II, respectively, in sludge-amended soil with different initial DEHP concns. Aerobic $t_{1/2}$ = 37 d and 51 d for phase I and II in well mixed sludge, $t_{1/2}$ = 120 d and > 365 d for phase I and II in aggregate sludge, $t_{1/2}$ = 55 d and 150 d for phase I and II in sludge-amended soil; anaerobic $t_{1/2}$ = 301 d and > 365 d for phase I and II in sludge-amended soil (laboratory microcosms, Madsen et al. 1999)

biodegradation in aerobic soil: $t_{1/2}$ = 2.0 – 69.3 d in various sand, loam, soils with different organic carbon content and sludge amended loam in laboratory and outdoor experiments (Peterson & Staples 2003)

Biota: elimination and degradation $t_{1/2}$ < 4 d after 7 d for water fleas *Daphnia magna* and $t_{1/2}$ = 7 d for fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2}$ = 12.2 d (fathead minnows *Pimephales promelas*, Mayer 1976);

depuration $t_{1/2}$ = 3 d (in tissues of bluegill sunfish continuously for 42-d exposure, Barrows et al. 1980)

depuration $t_{1/2}$ = 38 d from sheephead minnow (Karara & Hayton 1984).

TABLE 15.1.3.13.1

Reported vapor pressures of *bis*(2-ethylhexyl) phthalate (DEHP) 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)		

OECD 1981		OECD 1993		Goodman 1997			
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
effusion-vapor pres. balance				orifice diameter 0.381 mm		orifice diameter 0.0229 mm	
10	1.1×10^{-6}	40	1.2×10^{-4}	50	1.2×10^{-4}	using variable cell height	
20	6.0×10^{-6}	50	4.8×10^{-4}	50	3.1×10^{-4}	50	2.1×10^{-4}
30	2.8×10^{-5}	55	9.3×10^{-4}	55	9.8×10^{-4}	60	9.7×10^{-4}
40	1.2×10^{-4}	60	1.8×10^{-3}	55	6.5×10^{-4}	65	4.1×10^{-3}

(Continued)

TABLE 15.1.3.13.1 (*Continued*)

OECD 1981		OECD 1993		Goodman 1997			
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50	4.9×10^{-4}	65	3.3×10^{-3}	60	2.0×10^{-3}	70	6.8×10^{-3}
		70	5.9×10^{-3}	60	1.3×10^{-3}	75	9.2×10^{-3}
eq. 1	P/Pa	75	0.011	65	3.8×10^{-3}	80	1.0×10^{-2}
A	13.243	80	0.019	65	2.3×10^{-3}	40	1.2×10^{-4}
B	6035.017			70	6.3×10^{-3}	50	4.9×10^{-4}
				70	4.2×10^{-3}	60	1.5×10^{-3}
gas saturation				75	9.2×10^{-3}	70	4.6×10^{-3}
10	1.1×10^{-6}	**Small et al. 1948**		80	0.012	80	1.6×10^{-2}
20	6.0×10^{-6}	**effusion method**					
30	2.8×10^{-5}	t/°C	P/Pa				
40	1.2×10^{-4}					eq. 1	P/Pa
50	4.9×10^{-4}	data presented in graph and				A	14.90
		eq. 1	P/mmHg			B	5911
eq. 1	P/Pa	A	12.47				
A	10.086	B	5757				
B	5010.357	for pressure range: 0.05 to					
			10^{-4} mmHg				
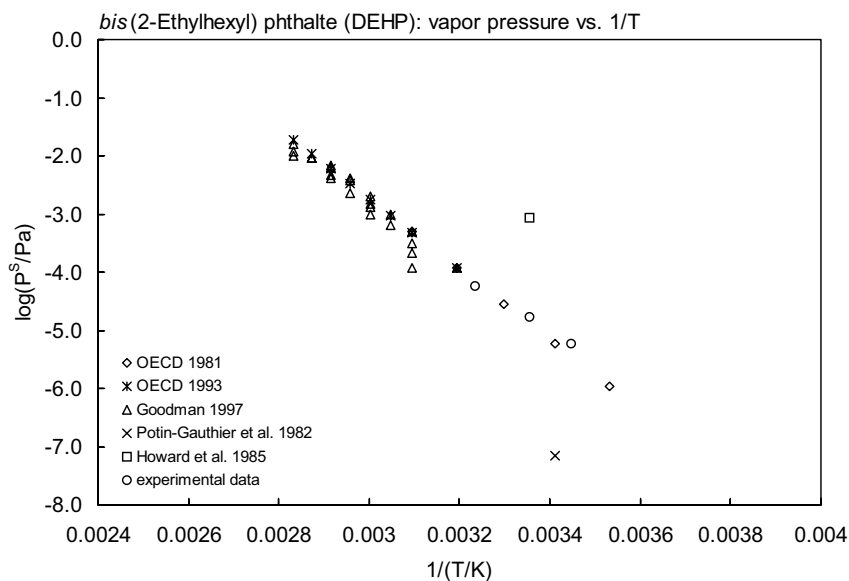
FIGURE 15.1.3.13.1 Logarithm of vapor pressure versus reciprocal temperature for *bis*(2-ethylhexyl) phthalate.

15.1.3.14 Di(hexyl,octyl,decyl) phthalate

Common Name: Di(hexyl,octyl,decyl) phthalate
Synonym: 610P
Chemical Name:
CAS Registry No: 25724-58-7, 68515-51-5
Molecular Formula: $C_{25}H_{40}O_4$
Molecular Weight: 404.583
Melting Point (°C):
    –4   (Staples et al. 1997)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
    547.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    0.9 ± 0.5   (shake flask, Howard et al. 1985)
    0.05; 0.0004 (recommended; calculated-QSAR, Staples et al. 1997)
    8.76×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
    6.5×10^{-4} (gas saturation, Howard et al. 1985)
    6.5×10^{-4}; 4.53×10^{-5}, 6.5×10^{-2} (recommended; calculated-QSAR, Staples et al. 1997)
    1.31×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    6.05   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.9–8.61   (HPLC-RT correlation, Howard et al. 1985; quoted, Staples et al. 1997)
    7.25; 8.54   (recommended; calculated-QSAR, Staples et al. 1997)
    8.17   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    10.78   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
    Volatilization:
    Photolysis:
    Oxidation: atmospheric photooxidation $t_{1/2}$ ~ 0.2–4.0 d (estimated, Staples et al. 1997).
    Hydrolysis:
    Biodegradation: primary biodegradation with a rate constant k = 0.131 d^{-1} and $t_{1/2}$ = 5.30 d in an acclimated
        shake flask CO_2 evolution test (Sugatt et al. 1984).
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2}$ ~ 0.2–4.0 d (estimated, Staples et al. 1997).

Surface water: primary biodegradation with a rate constant $k = 0.131$ d^{-1} and $t_{1/2} = 5.30$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.15 Diisononyl phthalate (DINP)
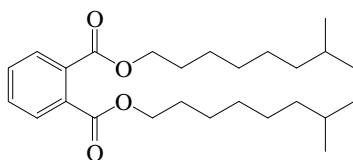
Common Name: Diisononyl phthalate
Synonym: DINP
Chemical Name:
CAS Registry No: 28553-12-0, 68515-48-0
Molecular Formula: $C_{26}H_{42}O_4$
Molecular Weight: 418.609
Melting Point (°C):
    –48   (Staples et al. 1997)
Boiling Point (°C):
    413   (Fishbein & Albro 1972)
Density (g/cm³ at 20°C):
    0.995   (Fishbein & Albro 1972)
Molar Volume (cm³/mol):
    569.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.20 ± 0.1   (shake flask-GC, Howard et al. 1985)
    0.20, 0.0006 (quoted, Staples et al. 1997)
    < 0.001; 7.8×10^{-5}, 2.3×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)
    3.08×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)
    6.1×10^{-4} (20°C, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C):
    7.2×10^{-5} (gas saturation method, Howard et al. 1985)
    6.67×10^{-5}; 1.33×10^{-8}, 3.07×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)
    6.81×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    9.26   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    > 8.0; 9.0, 9.4   (recommended; calculated-QSAR, Staples et al. 1997)
    8.60   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    11.03   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:
    3.27   (*Arca zebra*, Solbakken et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

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

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim$ 0.2–2.0 d (estimated, Staples et al. 1997).

k_{OH} = 23.408 × 10^{-12} cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.35 d based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant k = 0.131 d^{-1} and $t_{1/2}$ = 5.31 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

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

k_1 = 848 mL·g·d^{-1} (*Arca zebra*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

k_2 = 0.46 d^{-1} (*Arca zebra*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

k_2 = 0.02 d^{-1} (*Diplora strigosa*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim$ 0.2–2.0 d (estimated, Staples et al. 1997).

Photodegradation $t_{1/2}$ = 0.35 h based on a global, seasonal and diurnal average OH radical concn of 1 × 10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: primary biodegradation with a rate constant k = 0.131 d^{-1} and $t_{1/2}$ = 5.31 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.16 Di-isodecyl phthalate (DIDP)
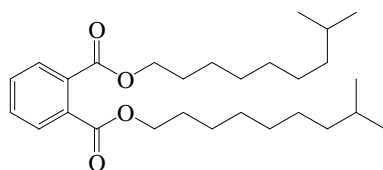
Common Name: Di-isodecyl phthalate
Synonym: DIDP
Chemical Name: di-diisodecyl phthalate
CAS Registry No: 26761-40-0, 68515-49-1
Molecular Formula: $C_{28}H_{46}O_4$
Molecular Weight: 446.663
Melting Point (°C):

    –48   (Stephenson & Malanowski 1987)
    –46   (Staples et al. 1997)
    –50   (Lide 2003)

Boiling Point (°C):

    450   (Stephenson & Malanowski 1987)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

    464.8   (Stephenson & Malanowski 1987)
    613.6   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

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

    < 50   (quoted from Monsanto Chemical Co. data sheets, Peakall 1975)
    1.19 ± 0.19 (shake flask-GC, Howard et al. 1985)
    0.28   (shake flask-nephelometry, Hollifield 1979)
    0.19, 0.28, < 0.00013 (quoted, Staples et al. 1997)
    < 0.001; 2.2×10^{-6}, 7.4×10^{-6} (recommended, calculated-QSAR, Staples et al. 1997)
    3.81×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)
    1.7×10^{-4} (20°C, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

    $\log (P_L/kPa) = 14.0158 - 10984/(242.24 + T/K)$, temp range: 371–496 K, (Antoine eq., Stephenson & Malanowski 1987)
    $\log (P/mmHg) = 81.7895 - 7.4225 \times 10^3/(T/K) - 26.916 \cdot \log (T/K) + 1.1502 \times 10^{-2} \cdot (T/K) - 4.353 \times 10^{-14} \cdot (T/K)^2$; temp range 233–723 K (vapor pressure eq., Yaw et al. 1994)
    6.67×10^{-5}, 7.47×10^{-5} (quoted, Staples et al. 1997)
    6.67×10^{-5}; 6.67×10^{-6}, 4.93×10^{-6}, 1.33×10^{-8} (recommended, calculated-QSAR, Staples et al. 1997)
    1.84×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

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

    21.6   (calculated-QSPR, Cousins & Mackay 2000)

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

    7.70   (estimated, Williams et al. 1995)
    > 8.0; 10.0, 1.0.3   (recommended; calculated-QSAR, Staples et al. 1997)
    9.46   (calculated-QSPR, Cousins & Mackay 2000)

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

    11.52   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

    1.95–2.1, 2.06   (*Daphnia magna*, 20°C, range, mean, Brown & Thompson 1982a)
    3.48, 3.60; 3.54   (*Mytilus edilus*, 15°C, exposure concn: 4.4, 4.17 µg/L; mean value, Brown & Thompson 1982b)

Sorption Partition Coefficient, log K_{OC}:

    5.04, 5.78, 5.16   (soil/sediment, exptl. data, Williams et al. 1995)
    5.46, 7.60   (soil/sediment: mean value, calculated-K_{OW}, Williams et al. 1995)

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

    Volatilization:
    Photolysis:
    Oxidation: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997).
        k_{OH} = 26.217 × 10^{-12} cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.32 d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)
    Hydrolysis:
    Biodegradation: degradation $t_{1/2}$ = 4.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);
        primary biodegradation with a rate constant k = 0.088 d^{-1} and $t_{1/2}$ = 9.6 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).
   Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
        k_1 = 795, 539 mL·g·d^{-1} (*Mytilus edilus*, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).
        k_2 = 0.20, 0.18 d^{-1} (*Mytilus edilus*, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

Half-Lives in the Environment:

    Air: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997).
        photodegradation $t_{1/2}$ = 0.32 d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)
    Surface water: primary biodegradation with a rate constant k = 0.088 d^{-1} and $t_{1/2}$ = 9.6 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).
    Groundwater:
    Sediment:
    Soil: degradation $t_{1/2}$ = 4.0 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).
    Biota: depuration $t_{1/2}$ = 3.5 and 3.8 d DIDP concn at 5 and 50 µgL^{-1} for *Mytilus edilus* at 15°C (Brwon & Thompson 1982b).

15.1.3.17 Diundecyl phthalate (DUP)
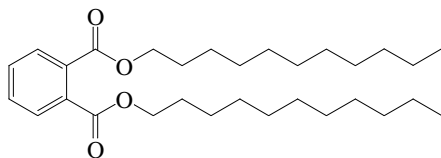
Common Name Diundecyl phthalate
Synonym: DUP
Chemical Name: diundecyl phthalate
CAS Registry No: 3648-20-2
Molecular Formula: $C_{30}H_{50}O_4$
Molecular Weight: 474.716
Melting Point (°C):
    –9   (Staples et al. 1997)
    35.5   (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
    0.96   (Staples et al. 1997)
Molar Volume (cm³/mol):
    658.0   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.789 (mp at 35.5°C)

Water Solubility (g/m³ or mg/L at 25°C):
    1.11 ± 0.28   (shake flask, Howard et al. 1985)
    < 0.001; 1.6×10^{-7}, 4.2×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)
    2.14×10^{-8} (calculated-UNIFAC, Thomsen et al. 1999)
    4.41×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
    6.67×10^{-5}, 7.07×10^{-5} (quoted, Staples et al. 1997)
    6.67×10^{-5}; 1.33×10^{-8}, 1.6×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)
    4.97×10^{-7} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    50.5   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    > 8.0; 11.2, 11.5   (recommended; calculated-QSAR, Staples et al. 1997)
    10.54   (calculated-UNIFAC, Thomsen et al. 1999)
    10.33   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    12.02   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

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

Oxidation: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997).

$k_{OH} = 31.847 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $t_{1/2}$ = 0.26 d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation rate constant k = 0.115 d^{-1} and $t_{1/2}$ = 6.17 d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

aerobic biodegradation in aquatic environments, first order k = 0.03 d^{-1} with $t_{1/2}$ = 23 d in unstirred river water (Peterson & Staples 2003)

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997)

Photodegradation $t_{1/2}$ = 0.26 d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant k = 0.115 d^{-1} and $t_{1/2}$ = 6.17 d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984).

biodegradation $t_{1/2}$ - 23 d in aerobic aquatic environments (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.18 Ditridecyl phthalate (DTDP)
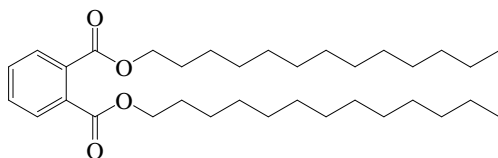
Common Name: Ditridecyl phthalate
Synonym: DTDP
Chemical Name:
CAS Registry No: 119-06-2. 68515-47-9
Molecular Formula: $C_{34}H_{58}O_4$
Molecular Weight: 530.823
Melting Point (°C):
    −37   (Staples et al. 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C):
    0.953   (Staples et al. 1997)
Molar Volume (cm³/mol):
    746.8   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    0.34   (shake flask-nephelometry, Hollifield 1979)
    < 0.30   (shake flask, Howard et al. 1985; quoted, Adams et al. 1995)
    0.34, < 0.30 (quoted, Staples et al. 1997)
    < 0.001; 1.5×10^{-9}, 4.2×10^{-9} (recommended, calculated-QSAR, Staples et al. 1997)
    4.07×10^{-10} (calculated-UNIFAC, Thomsen et al. 1999)
    7.0×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C):
    $< 6.67 \times 10^{-5}$ (quoted, Staples et al. 1997)
    $< 6.67 \times 10^{-5}$; 1.33×10^{-9}, 3.33×10^{-9} (recommended; calculated-QSAR, Staples et al. 1997)
    3.63×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    275   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
    8.40   (estimated, Williams et al. 1995)
    > 8.0; 13.1, 13.4   (recommended; calculated-QSAR, Staples et al. 1997)
    12.28   (calculated-UNIFAC, Thomsen et al. 1999)
    12.06   (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
    13.01   (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
    6.08   (soil/sediment, Williams et al. 1995; quoted, Staples et al. 1997)

5.87, 6.45, 6.28; 6.08 (soil/sediment: exptl. data; mean value, Williams et al. 1995)

6.26, 8.30   (soil/sediment: exptl. mean, calculated-K_{OW}, Williams et al. 1995)

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

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2}$ = 10.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation rate constant k = 0.029 d^{-1} and $t_{1/2}$ = 27.6 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2}$ ~ 0.2–2.0 d (estimated, Staples et al. 1997).

Surface water: primary biodegradation rate constant k = 0.029 d^{-1} and $t_{1/2}$ = 27.6 d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation $t_{1/2}$ = 10.5 d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.19 Butyl benzyl phthalate (BBP)
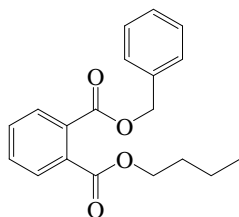
Common Name: Butyl benzyl phthalate
Synonym: BBP, benzyl butyl phthalate
Chemical Name: butyl benzyl phthalate, benzyl butyl phthalate
CAS Registry No: 85-68-7
Molecular Formula: $C_{19}H_{20}O_4$, $C_6H_5COOCH_2C_6H_4COOC_4H_9$
Molecular Weight: 312.360
Melting Point (°C):
    –35.0   (Callahan et al. 1979; Mabey et al. 1982; Howard 1989)
Boiling Point (°C):
    370.0   (Verschueren 1983; Howard 1989; Lide 2003)
Density (g/cm³ at 20°C):
    1.111   (Staples et al. 1997)

Molar Volume (cm³/mol):
    369.2   (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
    2.90   (Hirzy et al. 1978)
    0.71   (shake flask-nephelometry, practical grade, Hollifield 1979)
    2.9 ± 1.2   (shake flask-GC, Gledhill et al. 1980)
    40.2   (shake flask-LSC, Veith et al. 1980)
    2.82   (20°C, shake flask-UV, Leyder & Boulanger 1983)
    2.90 ± 1.2 (Verschueren 1983)
    2.69 ± 0.15 (shake flask-HPLC/UV, Howard et al. 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    0.00115   (20°C, Gledhill et al. 1980)
    0.00799   (calculated using Truton's rule, Mabey et al. 1982)
    0.00115   (Petrasek et al. 1983)
    0.00115   (20°C, Verschueren 1983)
    log $(P_L$/kPa) = 9.1472 – 4647.5/(T/K), temp range: 416–516 K, (Antoine eq., Stephenson & Malanowski 1987)
    0.0011, 0.00133   (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
    0.00067   (recommended, Staples et al. 1997)
    0.0249   (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.132   (calculated-P/C, Wolfe et al. 1980a)
    0.132   (calculated, Lyman et al. 1982)
    0.841   (calculated-P/C, Mabey et al. 1982)
    0.104   (quoted from WERL Treatability Data, Ryan et al. 1988)
    0.077   (selected, Staples et al. 1997)
    0.205   (calculated-QSPR, Cousins & Mackay 2000)

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

4.80	(Hirzy et al. 1978)
5.80	(calculated as per Leo et al. 1971)
4.77	(shake flask-GC analysis of both phases, Gledhill et al. 1980)
4.05	(shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
4.75	(RPHPLC-RT correlation, Veith et al. 1980)
3.97	(HPLC-k′ correlation, McDuffie 1981)
4.11, 3.23–4.45	(shake flask method: mean, range, OECD 1981)
4.91	(20°C, shake flask-UV, Leyder & Boulanger 1983)
4.78	(Verschueren 1983)
3.57	(HPLC-RT correlation, Howard et al. 1985)
4.91	(calculated, Hansch & Leo 1985)
4.87	(calculated-CLOGP, Müller & Klein 1992)
4.59	(recommended, Staples et al. 1997)
4.70	(calculated-QSPR, Cousins & Mackay 2000)

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

8.78	(calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

2.74–3.34	(calculated-K_{OW}, Veith et al. 1979, 1980)
2.82	(bluegill sunfish, Barrows et al. 1980;)
2.71	(calculated-K_{OW}, Gledhill et al. 1980)
2.82	(bluegill sunfish, quoted, Gledhill et al. 1980)
2.19–2.95	(fathead minnows, quoted, Gledhill et al. 1980)
2.89	(bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
3.90	(calculated-K_{OW}, Wolfe et al. 1980a)
4.67	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
3.57	(sediment, calculated-K_{OW}, Pavlou & Weston 1983, 1984)
2.89	(quoted, Isnard & Lambert 1988; quoted, Banerjee & Baughman 1991)
2.72	(calculated-K_{OW} and $S_{octanol}$, Banerjee & Baughman 1991)

Sorption Partition Coefficient, log K_{OC}:

1.83–2.54	(soil, batch equilibration-GC, Gledhill et al. 1980;)
3.95	(soil/sediment, Gledhill et al. 1980)
3.81	(calculated-K_{OW}, Wolfe et al. 1980a)
5.23	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
4.23	(Broome County soil in New York, Russell & McDuffie)
4.23, 3.97	(soil, quoted, calculated-MCI and fragment contribution, Meylan et al. 1992)
2.60	(activated carbon, calculated-MCI, Blum et al. 1994)
3.21	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
5.00	(suspended solids, calculated-K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)
3.21, 3.88; 3.11, 3.07, 3.21, 3.32, 3.15	(soil: quoted lit., calculated-K_{OW}; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

Volatilization:

Photolysis: direct photolysis (near surface) rate constant k = 2×10^{-4} h^{-1} in natural water (Wolfe et al 1980a); photodegradation $t_{1/2}$ > 100 d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989).

Oxidation: the free radical oxidation rate constant k = 18 M·s^{-1} for reaction with peroxy radical (Wolfe et al. 1980a);

rate constant k << 360 M^{-1}·h^{-1} for singlet oxygen and k = 280 M^{-1}·h^{-1} for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2}$ = 6–60 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

predicted atmospheric photooxidation $t_{1/2} = 0.5$–5.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).

$k_{OH} = 11.049 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} and $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis: the alkaline hydrolysis rate constant k ~ 38 M^{-1}·h^{-1}; hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

chemical degradation (hydrolysis) $t_{1/2} > 100$ d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989; selected, Staples et al. 1997).

Biodegradation: degradation $t_{1/2}$ ~ 2 d in river water and $t_{1/2} = 2$ h in activated sludge (Saeger & Tucker 1976)

degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

microbial degradation rate constant k = 2.9×10^{-8} mL·organism^{-1}·s^{-1} (Wolfe et al. 1981a);

0–24% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

primary degradation accounted for > 95% loss in 7 d with an initial concentration of 1.0 mg/L in a lake water microcosm with $t_{1/2} = < 4$ d and 100% primary degradation was observed after 9 d while $t_{1/2} = 2.0$ d (Gledhill et al. 1980; quoted, Verschueren 1983; Howard 1989);

significant degradation with rapid adaptation within 7 d in an aerobic environment with k > 0.5 d^{-1} (Tabak et al. 1981; quoted, Mills et al. 1982);

degradation rate constant k = 0.043 d^{-1} corresponding to $t_{1/2} = 19.4$ d in a shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% degraded within 40 d in digested sludge (Shelton et al. 1984);

99% degraded in activated sludge systems in 48 h (O'Grady et al. 1985);

anaerobic digestion of sludge with first-order rate constant k = 6.5×10^{-3} h^{-1} and $t_{1/2} = 107$ h (Ziogou et al. 1989);

aqueous aerobic $t_{1/2} = 24$–168 h, based on unacclimated river die-away test and aqueous anaerobic $t_{1/2} = 672$–4320 h, based on unacclimated anaerobic screening test data (Howard et al. 1991)

Aerobic biodegradation in aquatic environments, first order k = 0.46 d^{-1} with $t_{1/2} = 1.5$ d in unstirred river water, k = 0.50 d^{-1} with $t_{1/2} = 1.4$ d in microcosm, lake, k = 0.35 d^{-1} with $t_{1/2} = 2.0$ d in river water, k = 0.14 d^{-1} with $t_{1/2} = 5.0$ d in microcosm, un-impacted, k > 0.023 d^{-1} with $t_{1/2} < 3.0$ d in microcosm, Illinois river, and k = 2.2 d^{-1} with $t_{1/2} = 0.32$ d in shake river water (Peterson & Staples 2003)

Anaerobic biodegradation k = 0.056 d^{-1} with $t_{1/2} = 12.4$ d in undiluted sludge, batch incubation, k = 0.19 d^{-1} with $t_{1/2} = 3.7$ d in undiluted sludge, k = 0.096 d^{-1} with $t_{1/2} = 7.2$ d in 10% dilute sludge; k = 0.076 d^{-1} with $t_{1/2} = 9.1$ d in 10% freshwater sediment and k = 0.051 d^{-1} with $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: estimated rate constant k = 3×10^{-9} mL·cell^{-1}·h^{-1} for bacterial transformation in water (Mabey et al. 1982);

microbial transformation k = $(3.1 \pm 0.8) \times 10^{-11}$ L·organism^{-1}·h^{-1} in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

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

depuration $t_{1/2} < 24$ and > 48 h from tissues of bluegill sunfish (Barrows et al. 1980).

k_2 = 0.0464 d^{-1} (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

k_2 = 0.00397 d^{-1} (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.5$ d in the atmosphere (GEMS 1984; quoted, Howard 1989);

$t_{1/2} = 6$–60 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2}$ ~ 2 h by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);

hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

$t_{1/2} = 2$ d for river water, $t_{1/2} < 4$ d for lake water-sediment microcosm, and $t_{1/2} < 100$ d for chemical degradation (hydrolysis) (Gledhill et al. 1980);

biodegradation $t_{1/2} = 19.4$ d in an acclimated shake flask CO$_2$ evolution test (Sugatt et al. 1984);

overall $t_{1/2}$ = 24–168 h, based on unacclimated river die-away test (Howard et al. 1991)

biodegradation $t_{1/2}$ = 0.32–3 d in aerobic aquatic environments (Peterson & Staples 2003)

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

Sediment: anaerobic biodegradation $t_{1/2}$ = 9.1 h in 10% freshwater sediment, and $t_{1/2}$ = 13.6 d in 10% salt marsh sediment (Peterson & Staples 2003)

Soil: degradation $t_{1/2}$ = 3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2}$ = 10–50 d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

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

Biota: depuration $t_{1/2}$ < 24 and > 48 h (tissues of bluegill sunfish in 21-d exposure, Barrows et al. 1980)

$t_{1/2}$ < 2 d from bluegill sunfish (Gledhill et al. 1980; quoted, Verschueren 1983).

15.1.4 PHOSPHATE ESTERS

15.1.4.1 Triaryl phosphates

15.1.4.1.1 t-Butylphenyl diphenyl phosphate (tBPDP, BPDP)
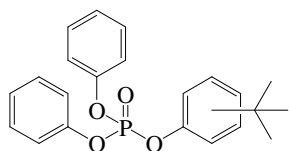
Common Name: *t*-Butylphenyl diphenyl phosphate
Synonym: TBPDP, BPDP
Chemical Name:
CAS Registry No: 56803-37-3
    o-tert-butylphenyl diphenyl phosphate (*o*-TBPDP)   83242-23-2
    m-tert-butylphenyl diphenyl phosphate (*m*-TBPDP)   83242-22-2
    p-tert-butylphenyl diphenyl phosphate (*p*-TBPDP)   981-40-8
Molecular Formula: $C_{22}H_{23}O_4P$, $(CH_3)C_6H_4(C_6H_5)_2O_4P$
Molecular Weight: 382.389
Melting Point (°C):
    –21   (Muir 1984)
Boiling Point (°C):
    195/0.20 mmHg, 200/0.2 mmHg, 200/0.20 mmHg (*o*-, *m*-, *p*-TBPDP, Wightman & Malaiyanki 1983)
    261/6 mmHg   (Muir 1984)
    420   (Boethling & Cooper 1985)
Density (g/cm³):
Molar Volume (cm³/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):
    3.2   (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):
    180   (200°C, Muir 1984)
    1.87×10^{-4} (quoted measured value, Boethling & Cooper 1985)
    6.13×10^{-5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.086   (estimated-P/C, Muir 1984, Muir et al. 1985)
    0.0223, 0.0073   (calculated-P/C, Boethling & Cooper 1985)
    2.18   (gas stripping, Muir et al. 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.12   (shake flask-concn ratio, Saeger et al. 1979;)
    3.23, 4.76, 6.44; 5.97   (RP-HPLC-k′ correlation; mean value, Renberg et al. 1980)

Bioconcentration Factor, log BCF:
    2.89   (calculated, Saeger et al. 1979)
    3.36, 3.04, 3.13   (rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)
    2.89   (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
    3.52, 2.89, 2.70   (fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
    2.76   (fathead minnow, calculated with hexane extract, Muir et al. 1983b)

3.94, 2.89 (rainbow trout, fathead minnow, static expt., quoted, Boethling & Cooper 1985)
3.64   (calculated-K_{OW}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
4.16   (calculated-K_{OW}, Muir 1984)
3.36   (soil, estimated from solubility, Boethling & Cooper 1985)

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

Volatilization: $t_{1/2}$ = 128 d from 1 m deep water system was estimated to be 128 d (calculated, Muir 1984) moderate rate of volatilization from water, $t_{1/2}$ = 152 d at 0.5-m depth (Muir et al. 1985).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2}$ = 1.92 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

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

k_1 = 22.8 h^{-1}, 29.3 h^{-1} (rainbow trout, exposure concn 5, 50 μg/L, Muir et al. 1983b).
k_1 = 17.7 h^{-1}, 18.0 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L, Muir et al. 1983b).
k_2 = 0.0137 h^{-1}, 0.0113 h^{-1} (rainbow trout, exposure concn 5, 50 μg/L for 0–144 h interval, Muir et al. 1983b).
k_2 = 0.0106 h^{-1}, 0.0111 h^{-1} (rainbow trout, exposure concn 5, 50 μg/L for 0–432 h interval, Muir et al. 1983b)
k_2 = 0.0088 h^{-1}, 0.0074 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L for 0–144 h interval, Muir et al. 1983b).
k_2 = 0.0078 h^{-1}, 0.0070 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L for 0–432 h interval, Muir et al. 1983b)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
hydrolysis $t_{1/2}$ = 1.92 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);
$t_{1/2}$ = 128 d, volatilization from 1 m deep water system (Muir 1984);
pseudo-first-order $t_{1/2}$ = 0.44 d in pond water; moderate rate of volatilization from water column with $t_{1/2}$ = 152 d at 0.5-m depth (Muir et al. 1985).

Groundwater:

Sediment: pseudo-first-order $t_{1/2}$ = 39 d in pond bottom sediment during a 49-d period (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2}$ = 42 h in chironomid larvae (Muir et al. 1985).

15.1.4.1.2   Cresyl diphenyl phosphate (CDP)
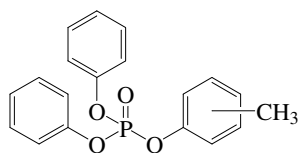
Common Name: Cresyl diphenyl phosphate
Synonym: CDP
Chemical Name:
CAS Registry No: 78-31-9
    o-CDP   5254-12-6
    m-CDP 69500-28-3
    p-CDP   78-31-9
Molecular Formula: $C_{19}H_{17}O_4P$
Molecular Weight: 340.309
Melting Point (°C):
    –40   (*p*-CDP, Lide 2003)
Boiling Point (°C):
    180/0.60 mmHg, 190/0.60 mmHg, 200/0.70 mmHg (*o*-, *m*-, *p*-CDP, Wightman & Malaiyandi 1983)
    368, 390   (at 1 atm, Boethling & Cooper 1985)
    235–255/4 mmHg, 255/5 mmHg (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
    2.60   (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):
    5.47×10^{-3}, 1.21×10^{-3}, 3.87×10^{-4}, 2.80×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)
    6.27×10^{-4} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.470   (calculated-P/C, Muir 1984)
    0.798, 0.162, 0.0820, 0.0507, 0.0355 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    4.505   (shake flask-concn ratio, Saeger et al. 1979)
    3.23, 3.63, 4.06; 3.77 (RP-HPLC-k′ correlation; mean value, Renberg 1980)
    4.40   (Bengtsson et al. 1986)

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

Bioconcentration Factor, log BCF:
    2.56   (calculated, Saeger et al. 1979)
    2.99   (calculated-K_{OW}, Boethling & Cooper 1985)
    2.002.34 (bleak, 280-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

    3.83   (calculated-K_{OW}, Muir 1984)

    3.41   (soil, estimated from solubility, Boethling & Cooper 1985)

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

    Volatilization: $t_{1/2}$ ~ 22 d for 1 m deep water system (estimated, Muir 1984).

    Photolysis:

    Oxidation:

    Hydrolysis:

    Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2}$ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

    Biotransformation:

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

Half-Lives in the Environment:

    Air:

    Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2}$ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

        volatilization $t_{1/2}$ = 22 d for 1 m deep water system (estimated, Muir 1984).

    Groundwater:

    Sediment:

    Soil:

    Biota: elimination $t_{1/2}$ = 4 d or less (beak, 28-d exposure, Bengtsson 1986).

15.1.4.1.3   Isopropylphenyl diphenyl phosphate (IPPDP)
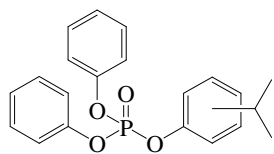
Common Name: Isopropylphenyl diphenyl phosphate
Synonym: IPPDP, IPDP
Chemical Name:
CAS Registry No: 28108-99-8
    o-IPPDP   64532-94-1
    m-IPPDP   69515-46-4
    p-IPPDP   55864-04-5
Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3)_2CHC_6H_4O_4P$
Molecular Weight: 368.362
Melting Point (°C):
    –26   (Muir 1984)
Boiling Point (°C):
    175/0.05 mmHg, 180/0.02 mmHg, 185/0.05 mmHg (Wightman & Malaiyandi 1983)
    220–230/1 mmHg   (Muir 1984, Boethling & Cooper 1985)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    2.20   (room temp, shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):
    1.47×10^{-4} (estimated from boiling point, Boethling & Cooper 1985)
    3.73×10^{-5} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    0.243, 0.0628   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.305   (shake flask-concn ratio, Saeger et al. 1979; quoted, Muir 1984)
    3.23, 4.30, 5.40, 6.57; 5.99   (RP-HPLC-k′ correlation; mean, Renberg et al. 1980)
    5.70   (quoted measured value, Boethling & Cooper 1985)

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

Bioconcentration Factor, log BCF:
    2.99   (calculated, Saeger et al. 1979)
    3.88   (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
    4.26   (calculated-K_{OW}, Muir 1984)
    3.45   (soil, estimated from solubility, Boethling & Cooper 1985)

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

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2}$ = 28–48 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ = 28–48 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Groundwater:

Sediment:

Soil:

Biota:

15.1.4.1.4   4-Cumylphenyl diphenyl phosphate (CPDPP)
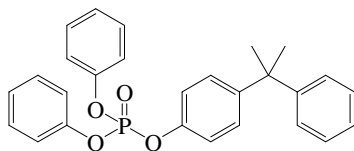
Common Name: 4-Cumylphenyl diphenyl phosphate
Synonym: CPDPP
Chemical Name:
CAS Registry No: 84602-56-2
Molecular Formula: $C_{27}H_{25}O_4P$, $C_6H_5C(CH_3)_2(C_6H_5)_2O_4P$
Molecular Weight: 444.458
Melting Point (°C):
Boiling Point (°C):
    230–235/0.15 mmHg (Wightman & Malaiyandi 1983)
    494   (Boethling & Cooper 1985)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
    0.063 ± 0.025   (Mayer et al. 1981)
    0.060   (Boethling & Cooper 1985)

Vapor Pressure (Pa at 25°C):
    1.726×10^{-9} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    8.62×10^{-4} (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    6.08   (Mayer at al. 1981)
    6.10   (quoted, Boethling & Cooper 1985)

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

Bioconcentration Factor, log BCF:
    3.40   (calculated-K_{OW}, Mayer et al. 1981)
    3.45, 3.10–3.66   (mean value, range, rainbow trout 90-d exposure, Mayer et al. 1981)
    4.40   (calculated-K_{OW}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
    4.53   (soil, calculated-S and K_{OW}, Mayer et al. 1981)
    4.30   (soil, estimated from solubility, Boethling & Cooper 1985)

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

Hydrolysis: hydrolyzed in alkaline solutions, $t_{1/2}$ = 5 d at pH 9 and 25°C, but $t_{1/2}$ > 28 d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: $t_{1/2}$ > 21 d in river die-away procedure; the half-lives of the disappearance by sediment adsorption and degradation of CPDFF for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2}$ < 3 d, sterile, aerated, light $t_{1/2}$ = 7 d and sterile, nitrogen-purge, light $t_{1/2}$ > 28 d (Mayer et al. 1981).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2}$ = 5 d at pH 9 and 25°C, but $t_{1/2}$ > 28 d at pH 5 and 7; biodegradation $t_{1/2}$ > 21 d in river die-away procedure (Mayer et al. 1981).

Groundwater:

Sediment: rapidly disappeared from the active core-water columns, 90% in < 3 d in the microcosm-lake simulation study, the half-lives of the disappearance of CPDFF by sediment adsorption and degradation are, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2}$ < 3 d; sterile, aerated, light $t_{1/2}$ = 7 d and sterile, nitrogen-purge, light $t_{1/2}$ > 28 d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.5   Nonylphenyl diphenyl phosphate (NPDPP)
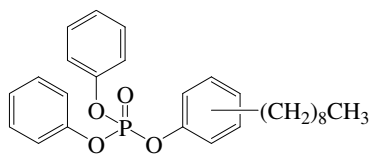
Common Name: Nonylphenyl diphenyl phosphate
Synonym: NPDPP, Pydral 50E
Chemical Name:
CAS Registry No: 38638-05-0
   m-NPDPP 84602-55-1
   p-NPDPP 64532-97-4
Molecular Formula: $C_{27}H_{33}O_4P$, $C_9H_{19}(C_6H_5)_3O_4P$
Molecular Weight: 452.522
Melting Point (°C):
Boiling Point (°C):
   220–225/0.07 mmHg (*m*-NPDPP, Wightman & Malaiyandi 1983)
   215–220/0.07 mmHg (*p*-NPDPP, Wightman & Malaiyandi 1983)
   471   (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
   0.77 ± 0.25 (Mayer et al. 1981)
   0.80   (Boethling & Cooper 1985)

Vapor Pressure (Pa at 2 5°C):
   6.13×10^{-5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):
   0.00142   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
   5.93   (Mayer et al. 1981; quoted, Muir 1984)
   5.90   (quoted, Boethling & Cooper 1985)

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

Bioconcentration Factor, log BCF:
   3.32   (estimated, Mayer et al. 1981)
   2.84, 2.49–2.96   (mean value and range, rainbow trout 90-d exposure, Mayer et al. 1981)
   4.26   (calculated-K_{OW}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
   4.36   (soil, calculated-solubility and K_{OW}, Mayer et al. 1981)
   4.61   (calculated-K_{OW}, Muir 1984)
   3.69   (soil, estimated from solubility, Boethling & Cooper 1985)

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

Oxidation:

Hydrolysis: $t_{1/2}$ = 6 d at pH 9 and 25°C, but $t_{1/2}$ > 28 d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: primary biodegradation $t_{1/2}$ > 21 d in river die-away procedure; half-life for disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2}$ < 3 d; sterile, aerated, light $t_{1/2}$ = 7 d and sterile, nitrogen-purge, light $t_{1/2}$ > 28 d (Mayer et al. 1981).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2}$ = 6 d at pH 9 and 25°C, but $t_{1/2}$ > 28 d at pH 5 and 7 (Mayer et al. 1981).

Groundwater:

Sediment: rapidly disappeared from the active core-water column, 90% in < 3 d. Time to 50% disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark – $t_{1/2}$ < 3 d; sterile, aerated, light – $t_{1/2}$ = 7 d and sterile, nitrogen-purge, light –$t_{1/2}$ > 28 d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.6 Triphenyl phosphate (TPP)
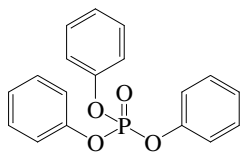
Common Name: Triphenyl phosphate
Synonym: TPP
Chemical Name: triphenyl phosphate
CAS Registry No: 115-86-6
Molecular Formula: $C_{18}H_{15}O_4P$
Molecular Weight: 326.283
Melting Point (°C):
  50.5   (Lide 2003)
Boiling Point (°C):
  245/11 mmHg (Verschueren 1983; Budavari 1989; Lide 2003)
  377   (Stephenson & Malanowski 1987)
Density (g/cm³):
Molar Volume (cm³/mol):
  270.7   (50°C, Stephenson & Malanowski 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.27, 0.292

Water Solubility (g/m³ or mg/L at 25°C):
  1.90   (shake flask-GC, Saeger et al. 1979)
  1.9 ± 0.2 (Mayer et al. 1981)
  0.73   (shale flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  < 13.3   (30°C, Verschueren 1983)
  2.0×10^{-4}, 1.6×10^{-4}, 1.07×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)
  log (P/kPa) = 8.195 – 4253/(T/K); temp range 275–410°C (Antoine eq., Stephenson & Malanowski 1987)
  log (P/mmHg) = 28.0972 – 5.6684 × 10³/(T/K) – 5.9768·log (T/K) – 3.1567 × 10⁻⁹·(T/K) + 1.0751 × 10⁻¹²·(T/K)²;
    temp range 323–687 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):
  0.168   (calculated-P/C, Muir 1984)
  0.0265, 0.0284, 0.018   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.63   (shake flask-concn ratio, Saeger et al. 1979)
  4.62   (Mayer et al. 1981)
  4.78   (shake flask-concn ratio, Sasaki et al. 1981)
  3.15   (RP-HPTLC-k′ correlation, Renberg et al. 1980)
  3.63–3.61 (literature average, Muir 1984)
  4.60, 4.70 (Boethling & Cooper 1985)
  3.90   (Bengtsson et al. 1986)

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

Bioconcentration Factor, log BCF or log K_B:
  2.45, 2.62   (quoted-rainbow trout data, calculated-K_{OW}, Saeger et al. 1979)
  2.22   (fathead minnow, mixed isomers, Veith et al. 1979)

3.41   (rainbow trout, rate constant ratio k_1/k_2, Muir et al. 1980)
3.29, 2.63, 2.58   (rainbow trout, calculated-K_{OW}, Muir et al. 1980)
3.02, 2.92, 2.00   (rainbow trout, calculated-S, Muir et al. 1980)
2.62   (rainbow trout, estimated from K_{OW}, Mayer et al. 1981)
2.43, 2.12–2.56   (mean value, range, rainbow trout in 90-d exposure, Mayer et al. 1981)
2.40–2.79   (killifish, whole fish basis, 72-h exposure, static system, Sasaki et al. 1981)
2.04–2.18   (goldfish, static system, Sasaki et al. 1981; quoted, Boethling & Cooper 1985)
2.20–2.79   (killifish, flow through system, Sasaki et al. 1982; quoted, Boethling & Cooper 1985)
2.28–2.29   (killifish, 32–35 d exposure, flow through system, Sasaki et al. 1983)
3.14, 2.76, 2.96   (rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)
2.51   (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.24, 2.75, 2.34   (fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
2.62   (fathead minnow, calculated with hexane extract, Muir et al. 1983b)
2.76, 2.51   (rainbow trout in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
2.75, 2.62   (fathead minnow in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
3.26   (estimated-K_{OW}, Boethling & Cooper 1985)
2.60   (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
3.74   (soil, calculated-S, K_{OW}, Mayer et al. 1981)
3.89   (calculated-K_{OW}, Muir 1984)
3.49   (calculated-solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 60 d (Muir 1984).
Photolysis:
Oxidation:
Hydrolysis:
   k = 0.0253 and 0.0227 L mol^{-1} s^{-1} for the colorimetric and acid-base method, respectively, in dioxan-water (3:1 v/v) at 35°C; the mean second order rate constants: $10^3 k_2$ at 0°C, 10.1°C, 24.7°C, and 35°C were 0.235, 0.477, 1.06, and 2.32 L mol^{-1} s^{-1}, respectively, in 60% dioxan-water (Barnard et al. 1961);
   $t_{1/2}$ = 1.3 yr under neutral conditions from kinetic data in the environment (estimated, Saeger et al. 1979)
   k = 6.0×10^{-8} s^{-1}, with $t_{1/2}$ = 130 d, the pseudo-first-order rate constant in dioxan-water (3:1 v/v) at 100°C; while the second-order rate constant k = 0.0106 L mol^{-1} s^{-1} with $t_{1/2}$ = 23 d at pH 9.5 and $t_{1/2}$ = 474 d at pH 8.2 under alkaline conditions at 24.7°C (quoted, Howard & Deo 1979);
   k(second order alkaline) = 0.027 M^{-1} s^{-1}, with an estimated $t_{1/2}$ ~ 1000 yr (Wolfe 1980)
   $t_{1/2}$ = 19 d at pH 7 but $t_{1/2}$ = 3 d at pH 9 at 25°C, the most important process for abiotic transformation of aryl phosphates in the environment, much more rapid at alkaline than at neutral pH (Mayer et al. 1981, quoted, Boethling & Cooper 1985)
   $t_{1/2}$ = 7.5 d at pH 8.2, $t_{1/2}$ = 1.3 d at pH 9.5, $t_{1/2}$ = 20–25 d at pH 7 and 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985)
   $t_{1/2}$ = 0.49 h at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b)
Biodegradation: complete primary degradation in less than 7 d in the river die-away studies exposed to the natural microbial population of the river water; $t_{1/2}$ < 7 d for primary biodegradation rate for from semicontinuous activated sludge studies (Saeger et al. 1979);
   readily biodegraded, in the semicontinuous activated sludge test, degradation of TPP exceeding 95% was observed over a 24-h cycle, and river die-away tests showed $t_{1/2}$ = 2–4 d; time to 50% from the active core water-column disappearance for TPP in microcosms simulating lake conditions was 3–10 d (Mayer et al. 1981).
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
   k_1 = 46.36 h^{-1} (rainbow trout, Muir et al. 1980).
   k_2 = 0.0197 h^{-1} (rainbow trout, 0–9 d, fast clearance, Muir et al. 1980).
   k_2 = 0.00245 h^{-1} (rainbow trout, 9–31 d, slow clearance, Muir et al. 1980)

k_1 = 0.4–0.6 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 2.1–4.2 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 3.3–10.4 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 3.3–16.9 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.023 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, calculated by concn decay curve, Muir et al. 1983)

k_2 = 0.039 h^{-1} (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.011 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.016 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983).

k_1 = 22.7 h^{-1}, 20.7 h^{-1} (rainbow trout, exposure concn 5, 50 μg/L, Muir et al. 1983b).

k_1 = 16.5 h^{-1}, 14.5 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L, Muir et al. 1983b).

k_2 = 0.0116 h^{-1}, 0.0144 h^{-1} (rainbow trout, exposure concn 5, 50 μg/L for 0–432 h interval, Muir et al. 1983b)

k_2 = 0.0121 h^{-1}, 0.0140 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L for 0–144 h interval, Muir et al. 1983b).

k_2 = 0.0076 h^{-1}, 0.0107 h^{-1} (fathead minnow, exposure concn 5, 50 μg/L for 0–432 h interval, Muir et al. 1983b)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

$t_{1/2}$ = 5 h in the water containing killifish and over 100 h for goldfish (Sasaki et al. 1981);

hydrolysis $t_{1/2}$ = 19 d at pH 7 but $t_{1/2}$ = 3 d at pH 9; $t_{1/2}$ = 2–4 d in river die-away test at 25°C, (Mayer et al. 1981, quoted, Boethling & Cooper 1985);

$t_{1/2}$ = 7.5 d at pH 8.2 and $t_{1/2}$ = 1.3 d at pH 9.5, $t_{1/2}$ = 20–25 d at pH 7 at 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985);

estimated hydrolysis $t_{1/2}$ ~ 10^3 yr (Wolfe 1980);

volatilization $t_{1/2}$(calc) = 60 d for 1 m deep water(Muir 1984).

Ground water:

Sediment: water-column disappearance $t_{1/2}$ ~ 3 d of TPP by both adsorption and degradation from microcosms-lake simulation study, for the microcosm core conditions: active, aerated, light or dark – $t_{1/2}$ = 3 d; active, nitrogen-purge, light – $t_{1/2}$ = 3 d; sterile, aerated, light – $t_{1/2}$ = 7 d and sterile, nitrogen-purge, light – $t_{1/2}$ = 10 d (Mayer et al. 1981).

Soil:

Biota: elimination $t_{1/2}$ = 30.4 h in pond sediment-water, $t_{1/2}$ = 17.6 h in river water, $t_{1/2}$ = 62.7 h in river sediment-water, $t_{1/2}$ = 44.4 in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983a);

elimination $t_{1/2}$ = 4 d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.1.7   Tricresyl phosphate (TCP)
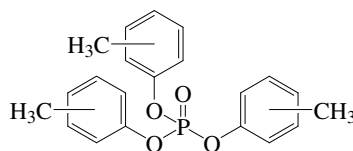
Common Name: Tricresyl phosphate
Synonym: TCP, tritolyl phosphate, tris(methylphenyl) phosphate
Chemical Name: phosphoric acid tris(methylphenyl) ester
     o-TCP:- *tris*(2-methylphenyl) phosphate; phosphoric acid tri(2-tolyl) ester
     m-TCP:- *tris*(3-methylphenyl) phosphate; phosphoric acid tri(3-tolyl) ester
     p-TCP:- *tris*(4-methylphenyl) phosphate; phosphoric acid tri(4-tolyl) ester
CAS Registry No:
     o-TCP [78-30-8]; *m*-TCP[563-04-2]; *p*-TCP [78-32-0]
     mixed isomers - *tris*(methylphenyl) phosphate [1330-78-5]
Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3C_6H_4)_3O_4P$
Molecular Weight: 368.362
Melting Point (°C):
     –25/–30   (*o*-TCP, Verschueren 1983)
     –33   (mixed isomers, Riddick et al. 1986)
     11, 25-26, 77–8   (*o*-TCP, *m*-TCP, *p*-TCP, Muir 1984)
     11, 25, 77.5   (*o*-TCP, *m*-TCP, *p*-TCP, Stephenson & Malanowski 1987)
     11, 25.5, 77.5   (*o*-TCP, *m*-TCP, *p*-TCP, Lide 2003)
Boiling Point (°C):
     201/1 mmHg(commercial quality, Burrow 1946)
     420   (*o*-TCP, Verschueren 1983)
     410   (*o*-TCP, Muir 1984: Lide 2003)
     313, 206, 216/0.5 mmHg (mixed isomers, *o*-, *m*-TCP, Riddick et al. 1986)
     241–255/4 mmHg, 265/5 mmHg(Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
     1.159, 1.1718   (25°C, mixture of isomers, *o*-TCP, Riddick et al. 1986)
     1.16   (*o*-TCP, Verschueren 1983; Riddick et al. 1987; Budavari 1989)
Molar Volume (cm³/mol):
     308.1   (20°C, calculated-density, Stephenson & Malanowski 1987)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
     116.3, 102.9, 113   (*m*-TCP, Small et al. 1948)
     113.4   (*p*-TCP, Small et al. 1948)
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):
     0.40   (shake flask-GC, Saeger et al. 1979)
     0.074   (*p*-TCP practical grade, shake flask-nephelometry; Hollifield 1979)
     0.36   (mixed isomers, Muir 1984)
     < 0.10   (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other
     temperatures designated * are compiled at the end of this section):
     0.00516–0.00612* (*m*-TCP, Celluloid Corporation samples at 80°C, static and dynamic methods, measured range
          80–136°C, Verhoek & Marshall 1939)
     log (P/µmHg) = 15.886 – 6088/(T/K); temp range 80–136°C (*m*-TCP, Celluloid Corporation samples, static and
          dynamic methods, Verhoek & Marshall 1939)

0.0132* (m-TCP, Eastman Kodak Co. samples at 85.2°C, static and dynamic methods, measured range 85.2–126°C, Verhoek & Marshall 1939)

log (P/μmHg) = 13.982 – 5373/(T/K); temp range 85.2–126°C (m-TCP, Eastman Kodak Co. samples, static and dynamic methods, Verhoek & Marshall 1939)

0.0113* (p-TCP, 92°C, static and dynamic methods, measured range 92–145°C, Verhoek & Marshall 1939)

log (P/μmHg) = 15.223 – 5926/(T/K); temp range 92–145°C (p-TCP, static and dynamic methods, Verhoek & Marshall 1939)

4.13×10^{-4} (extrapolated from exptl. data, measured range 140–156°C, commercial quality, ebulliometry, Burrows 1946)

log (P/mmHg) = 12.69 – 5925/(T/K); temp range: ~ 100–150°C (Antoine eq. from exptl., effusion, technical grade, Small et al. 1948)

log (P/mmHg) = 12.89 – 6088/(T/K) (m-TCP, Antoine eq. from literature, Small et al. 1948)

log (P/mmHg) = 10.98 – 5373/(T/K) (m-TCP, Antoine eq. from literature, Small et al. 1948)

log (P/mmHg) = 12.22 – 5895/(T/K); temp range: 100–150°C (m-TCP, Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)

log (P/mmHg) = 12.22 – 5926/(T/K) (p-TCP, effusion, Antoine eq., Small et al. 1948)

log (P/μmHg) = 14.12 – 5480/(T/K); temp range 115–168°C (p-TCP, pendulum-tensimeter method, Perry & Weber 1949)

log (P/mmHg) = [–0.2185 × 20835.9/(T/K)] + 10.654252; temp range 154.6–313°C (tritolyl phosphate, Antoine eq., Weast 1972–73)

log (P/kPa) = 11.81 – 5925/(T/K) (mixed isomers, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 8.56 – 4535/(T/K) (o-TCP, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 10.67 – 5787/(T/K) (m-TCP, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 13.24 – 5480/(T/K) (p-TCP, Antoine eq., Riddick et al. 1986)

2.26×10^{-4} (o-TCP, Antoine eq., interpolated, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.565 – 4535/(T/K); temp range 293–700 K (o-TCP, Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 11.8856 – 6104.5/[(T/K) – 10.81]; temp range 398–530 K (m-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)

log (P_L/kPa) = 10.245 – 5480/(T/K); temp range 388–530 K (p-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)

3.07×10^{-4}, 1.25×10^{-4} (estimated from reported boiling points, Boething & Cooper 1985)

1.87×10^{-4} (quoted measured value, Boethling & Cooper 1985)

6.10×10^{-6} (liquid P_L, GC-RT correlation, Hinckley et al. 1990)

log (P/mmHg) = 21.1624 – 5.2756×10^3/(T/K) – 3.3565·log(T/K) + 8.666×10^{-6}·(T/K) – 2.9202×10^{-9}·(T/K)^2; temp range 428–566 K (o-TCP, vapor pressure eq., Yaws et al. 1994)

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

0.0218 (calculated-P/C, Muir 1984, Muir et al. 1985)

0.283, 0.172, 0.111 (calculated-P/C, Boethling & Cooper 1985)

8.38 (m-TCP, gas stripping, Muir et al. 1985)

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

3.42 (HPLC-RT correlation, Veith 1979)

5.11 (shake flask-concn ratio, Saeger et al. 1979)

4.30, 4.65; 4.50 (RP-HPTLC-k′ correlation, Renberg et al. 1980)

5.107–5.12 (Muir 1984)

5.10–5.30 (Bengtsson et al. 1986)

Bioconcentration Factor, log BCF:

5.505, 4.45, 3.57, 3.57, 3.46 (p-TCP, ecological magnification factors for alga, snail, mosquito, fish and *Daphnia*, Metcalf 1976)

2.88 (calculated for rainbow trout, Saeger et al. 1979)

2.22 (fathead minnow, 32-d exposure, Veith et al. 1979)

3.44, 3.15, 3.17 (p-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)

2.89   (*p*-TCP for rainbow trout, calculated with hexane extract, Muir et al. 1983b)
3.34, 2.97, 2.77   (*p*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
2.85   (*p*-TCP, fathead minnow, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.07, 2.89, 3.04   (*m*-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)
2.49   (*m*-TCP for rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.22, 2.77, 2.59   (*m*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
2.66   (*m*-TCP, fathead minnow, calculated with hexane extract, Muir et al. 1983b)
3.15, 2.89; 3.64   (rainbow trout: *p*-, *m*-TCP, static expt.; estimated-K_{OW}, Boethling & Cooper 1985)
2.60   (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
4.44   (calculated-K_{OW}, Muir 1984)
3.86   (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 496 d (estimated, Muir 1984).
Photolysis:
Oxidation:
Hydrolysis: $t_{1/2}$ = 73 d and 52 d at 22°C for aryl phosphates (75% TCP and 18% TXP) in demineralized and river water (Wagemann et al. 1974; quoted, Boethling & Cooper 1985);
    degradation $t_{1/2}$ = 3–4 d for *o*-, *m*-TCP and 5 d for *p*-TCP in Lake Ontario water (Howard & Dao 1979)
    second order alkaline hydrolysis rate constant k = 0.025 M^{-1} s^{-1} (estimated, *p*-TCP, Wolfe 1980)
    $t_{1/2}$ = 1.31 h, 1.66 h for *m*-TCP and *p*-TCP, respectively, at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b).
Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 For *p*-TCP:
    k_1 = 25.8 h^{-1} 21.8 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
    k_1 = 15.9 h^{-1}, 7.80 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
    k_2 = 0.0104 h^{-1}, 0.00963 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
    k_2 = 0.0106 h^{-1}, 0.0133 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).
    k_2 = 0.0096 h^{-1}, 0.0077 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
    k_2 = 0.0070 h^{-1}, 0.0095 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).
 For *m*-TCP:
    k_1 = 28.8 h^{-1}, 24.0 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
    k_1 = 18.2 h^{-1}, 12.2 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
    k_2 = 0.0242 h^{-1}, 0.0229 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
    k_2 = 0.0115 h^{-1}, 0.0149 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).
    k_2 = 0.0147 h^{-1}, 0.0117 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
    k_2 = 0.0085 h^{-1}, 0.0101 h^{-1} (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).

Half-Lives in the Environment:
Air:
Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 7 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
    degradation $t_{1/2}$ = 3–4 d for *o*-, *m*-TCP and $t_{1/2}$ = 5 d for *p*-TCP in Lake Ontario water (Howard & Dao 1979);
    $t_{1/2}$ = 1.66 h and 1.31 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);
    volatilization $t_{1/2}$(calc) = 296 d in 1 m deep water system (Muir 1984);

pseudo-first-order $t_{1/2}$ = 0.57 d in pond water; moderate volatilization from water column with $t_{1/2}$ = 84 d at 0.5-m depth (Muir et al. 1985).

Groundwater:

Sediment: $t_{1/2}$ = 39 d in bottom sediment of a small pond (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2}$ = 135 h in chironomid larvae (Muir et al. 1985);
elimination $t_{1/2}$ = 4 d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

TABLE 15.1.4.1.7.1
Reported vapor pressures of tricresyl phosphate 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)	

tri-*m*-cresyl phosphate				tri-*p*-cresyl phosphate	
Verhoek & Marshall 1939				Verhoek & Marshall 1939	
static and dynamic methods				static and dynamic methods	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
Celluloid Corp. samples		Eastman Kodak samples			
80	0.00612	85.2	0.0132	92.0	0.0113
80	0.00604	95.4	0.0333	100.0	0.0267
80	0.00516	105.6	0.0749	110.0	0.0653
90	0.0177	115.8	0.1773	119.0	0.180
100.2	0.0461	126.0	0.448	119.0	0.189
109.9	0.1233			123.5	0.281
110.5	0.1276	eq. 1	P/μmHg	124.0	0.283
114.0	0.212	A	13.982	125.0	0.249
114.0	0.208	B	5373	129.0	0.441
114.0	0.213			129.0	0.448
119.0	0.323	ΔH_V = 102.84 kJ/mol		134.0	0.668
120.0	0.315			134.5	0.696
120.7	0.316			135.0	0.600
124.0	0.492			145.0	1.560
124.0	0.504				
125.9	0.509			eq. 1	P/μmHg
128.8	0.739			A	15.223
129.0	0.785			B	5926
130.0	0.777				
131.0	0.809			ΔH_V = 113.43 kJ/mol	
136.2	1.352				
eq. 1	P/μmHg				
A	15.886				
B	6088				
ΔH_V = 116.54 kJ/mol					

FIGURE 15.1.4.1.7.1a Logarithm of vapor pressure versus reciprocal temperature for *tris*(*m*-cresyl) phosphate.
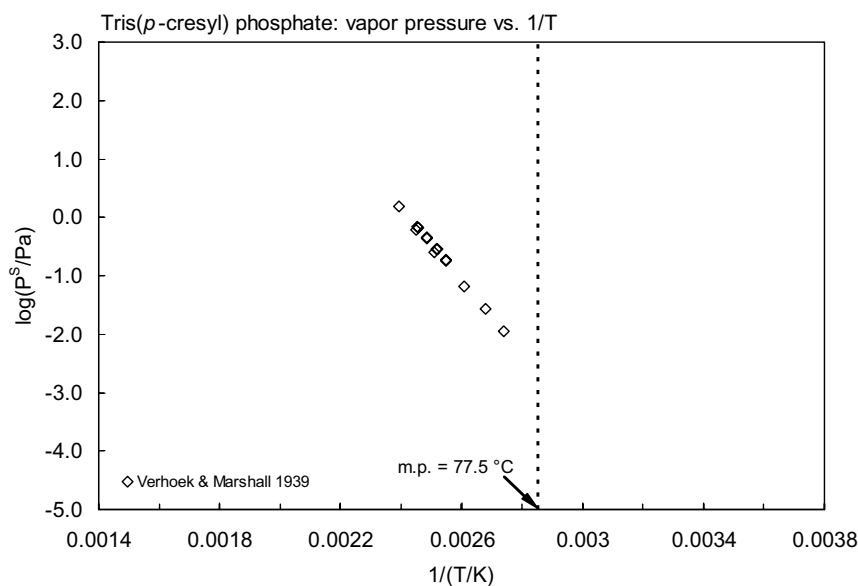
FIGURE 15.1.4.1.7.1b Logarithm of vapor pressure versus reciprocal temperature for *tris*(*p*-cresyl) phosphate.

15.1.4.1.8   Trixylenyl phosphate (TXP)
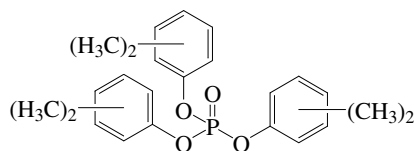
Common Name: Trixylenyl phosphate
Synonym: TXP
Chemical Name:
CAS Registry No: 25155-23-1
Molecular Formula: $C_{24}H_{27}O_4P$, $[(CH_3)_2C_6H_3]_3O_4P$
Molecular Weight: 410.442
Melting Point (°C):
    –20   (mixed isomers, Muir 1984)
Boiling Point (°C):
    261   (at 6 mmHg, Muir 1984)
    225–295/6 mmHg, 248–265/4 mmHg, 270/3 mmHg (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
    0.89   (shake flask-GC, Saeger et al. 1979)
    0.89   (mixed isomers, Muir 1984)

Vapor Pressure (Pa at 25°C):
    7.20×10^{-4}, 1.47×10^{-4}, 3.067×10^{-5} (estimated from reported boiling points, Boething & Cooper 1985)
    6.93×10^{-6} (30°C, Boething & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.334, 0.0689, 0.0142, 0.00314   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.63   (shake flask-concn ratio, Saeger et al. 1979)
    5.26   (RP-HPTLC-k′ correlation, Renberg et al. 1980)
    5.63   (Muir 1984)
    5.70   (Boethling & Cooper 1985)
    6.40–6.60   (Bengtsson et al. 1986)

Bioconcentration Factor, log BCF:
    3.15   (calculated for rainbow trout, Saeger et al. 1979)
    4.04   (estimated from K_{OW}, Boethling & Cooper 1985)
    3.11, 3.24, 3.28   (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
    4.44   (calculated-K_{OW}, Muir 1984)
    3.67   (estimated from solubility, Boethling & Cooper 1985)

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

   Volatilization:

   Photolysis:

   Oxidation:

   Hydrolysis:

   Biodegradation: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ = 28–48 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

   Biotransformation:

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

Half-Lives in the Environment:

   Air:

   Surface water: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ = 28–48 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

   Groundwater:

   Sediment:

   Soil:

   Biota: eliminated $t_{1/2}$ = 4 d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.2 Triaryl/alkyl phosphates

15.1.4.2.1 Dibutyl phenyl phosphate (DBPP)
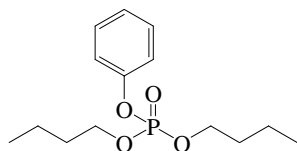
Common Name: Dibutyl phenyl phosphate
Synonym: DBPP
Chemical Name:
CAS Registry No: 2528-26-1
Molecular Formula: $C_{14}H_{23}O_4P$, $(C_4H_9)_2C_6H_5O_4P$
Molecular Weight: 286.303
Melting Point (°C):
Boiling Point (°C):
> 200/20 mmHg (Muir 1984)
> 155/2 mmHg, 155/1 mmHg (quoted, Boethling & Cooper 1985)
> Density (g/cm³):
> Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
> 96   (shake flask-GC, Saeger et al. 1979)

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):
> 66.7   (200°C, Muir 1984)
> 0.084, 0.0307   (estimated from boiling points, Boethling & Cooper 1985)
> 746*   (170°C, GC-RT correlation, measured range 170–200°C, Skene & Krzymien 1995)

Henry's Law Constant (Pa·m³/mol at 25°C):
> 0.253, 0.089   (estimated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
> 4.27   (shake flask-concn ratio, Saeger et al. 1979)
> 3.23   (RP-HPTLC-k′ correlation, Renberg et al. 1980)

Bioconcentration Factor, log BCF:
> 2.43   (calculated, Saeger et al. 1979)
> 3.04   (calculated-K_{OW}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
> 3.70   (calculated-K_{OW}, Muir 1984)
> 2.56   (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
> Volatilization: $t_{1/2}$ = 0.4 d (calculated, Muir 1984)
> Photolysis:
> Oxidation:
> Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} \sim 0.4$ d from 1 m deep water (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.2   2-Ethylhexyl diphenyl phosphate (EHDP)
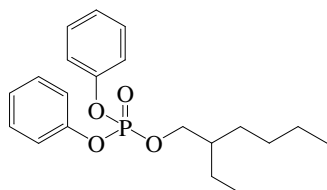
Common Name: 2-Ethylhexyl diphenyl phosphate
Synonym: EHDP
Chemical Name:
CAS Registry No: 1241-94-7
Molecular Formula: $C_{20}H_{27}O_4P$, $C_8H_{17}(C_6H_5)_2O_4P$
Molecular Weight: 362.399
Melting Point (°C):
    –80   (Muir 1984)
Boiling Point (°C):
    181/0.6 mmHg (Wightman & Malaiyandi 1983)
    239/1 mmHg (Muir 1984)
    150/0.2 mmHg, 375/760 mmHg, 230/5 mmHg (Boethling & Cooper 1985)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    1.9   (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):
    4.0×10^{-3}, 3.47×10^{-3}, 1.87×10^{-3} (estimated from reported boiling points, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    1.60   (calculated-P/C, Muir 1982, 1984)
    0.77, 0.648, 0.345   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.73   (shake flask-concn ratio, Saeger et al. 1979)
    5.00   (RP-HPLC-k′ correlation, Renberg et al. 1980)

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

Bioconcentration Factor, log BCF:
    3.20   (calculated, Saeger et al. 1979)
    3.17, 3.06; 3.12   (rainbow trout: calculated from rate constant ratio k_1/k_2 for exposure concn 5 and 50 μg/L;
        mean, Muir & Grift 1981)
    3.52   (calculated-K_{OW}, Muir & Grift 1981)
    4.11   (calculated-K_{OW}, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
    4.49   (calculated-K_{OW}, Muir 1984)
    3.49   (estimated from solubility, Boethling & Cooper 1985)

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

Volatilization: half-life for 1 m deep water was estimated to be 7 d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981).

Biotransformation:

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

$k_1 = 48.5$ h^{-1}, 33.0 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L, Muir & Grift 1981)

$k_2 = 0.0298$ h^{-1}, 0.0294 h^{-1} (rainbow trout, exposure concn 5, 50 µg/L, Muir & Grift 1981)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979;

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981);

volatilization $t_{1/2} \sim 7$ d for 1 m deep water (estimated, Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.3 Isodecyl diphenyl phosphate (IDDP)
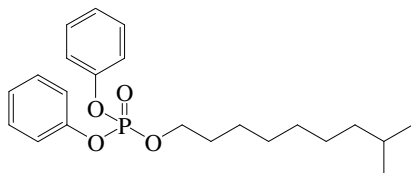
Common Name: Isodecyl diphenyl phosphate
Synonym: IDDP
Chemical Name:
CAS Registry No: 29761-21-5
Molecular Formula: $C_{22}H_{31}O_4P$, $C_{10}H_{21}(C_6H_5)_2O_4P$
Molecular Weight: 390.452
Melting Point (°C):
    < –50   (Muir 1984)
Boiling Point (°C):
    245/10 mmHg (Boethling & Cooper 1985)
Density (g/cm³ at 20°C):
Molar Volume (cm³/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):
    0.75   (room temp, shake flask-GC, Saeger et al. 1979)
    0.80   (Boethling & Cooper 1985)

Vapor Pressure (Pa at 25°C):
    < 13.33, 66.7   (100, 150°C, Muir 1984)
    2.133×10^{-3} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):
    12.97   (calculated-P/C, Muir 1984)
    1.013   (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:
    5.44   (shake flask-concn ratio, Saeger et al. 1979)
    3.31, 5.72; 5.42   (RP-HPTLC-k′ correlation; mean, Renberg et al. 1980)
    5.70   (quoted measured value, Boethling & Cooper 1985)

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

Bioconcentration Factor, log BCF:
    3.04   (calculated, Saeger et al. 1979)
    3.88   (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC}:
    4.33   (calculated-K_{OW}, Muir 1984)
    3.69   (soil, estimated from solubility, Boethling & Cooper 1985)

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

Volatilization: $t_{1/2}$ = 1.3 d for 1 m deep water system (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2}$ ~ 1.3 d for 1 m deep water system (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.4.3   Trialkyl phosphate

15.1.4.3.1   Tributyl phosphate (TBP)
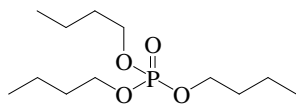
Common Name: Tributyl phosphate
Synonym: TBP, butyl phosphate
Chemical Name: tri-*n*-butyl phosphate
CAS Registry No: 126-73-8
Molecular Formula: $C_{12}H_{27}O_4P$; $(C_4H_9)_3O_4P$
Molecular Weight: 266.314
Melting Point (°C):
   < −80   (Dean 1985, Stephenson & Malanowski 1987)
Boiling Point (°C):
   289   (Lide 2003)
Density (g/cm³):
   0.972   (25°C, Dean 1992)
   0.976   (Riddick et al. 1986; Budavari 1989)
Molar Volume (cm³/mol):
   273.8   (Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
   14.67   (Dean 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
   422*   (shake flask-electrometric titration, measured range 3.4–50°C, Higgins et al. 1959)
   280   (shake flask-GC, Saeger et al. 1979)
   390   (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
   0.89   (extrapolated, Evans et al. 1930)
   0.10, 2.0   (114, 160.2°C, Riddick et al. 1986)
   log (P/kPa) = 7.7110 – 3206.5/(t/°C + 273) (Antoine eq., Riddick et al. 1986)
   log (P/kPa) = 7.7110 – 3206.5/(T/K) (Antoine eq., liquid phase, temp range 500–562 K, Stephenson & Malanowski 1987)
   0.0202   (estimated from average air-borne concn, Skene & Krzymien 1995)
   0.031, 0.015, 0.026, 0.030, 0.022   (extrapolated values from various reported Antoine equations, Skene & Krzymien 1995)
   0.149*   (gas saturation-GC, measured range 0–80°C; Skene & Krzymien 1995)
   log (P/Pa) = 8.85629 – 1690.26/(T/K – 123.431); temp range 0–80°C, (Antoine eq. derived from exptl. data, gas saturation-GC, Skene & Krzymien 1995)
   0.015   (TBP in Skydrol 500B-4 hydraulic fluid, gas saturation-GC, Skene & Krzymien 1995)
   927–1060*   (170°C, GC-RT correlation, measured range 170–200°C. Skene & Krzymien 1995)

Henry's Law Constant (Pa·m³/mol at 25°C):
   2513   (estimated-P/C, Muir 1984)

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

    4.004   (shake flask-concn ratio, Saeger et al. 1979)
    3.99   (Sasaki et al. 1981)
    4.004, 4.01 (quoted, Muir 1984)

Bioconcentration Factor, log BCF:

    2.28   (calculated, Saeger et al. 1979)
    1.49–1.54   (killifish, 90-h exposure, static water system, Sasaki et al. 1981)
    0.78–1.04   (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)
    0.602–1.43 (killifish, static water system, Sasaki et al. 1982)
    1.20–1.43   (killifish, 4–38 d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

    3.56   (calculated-K_{OW}, Muir 1984)

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

    Volatilization: $t_{1/2}$ = 0.4 d for 1 m deep water system (calculated, Muir 1984).
    Photolysis:
    Oxidation:
    Hydrolysis:
    Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).
    Biotransformation:
    Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

    Air:
    Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2}$ < 28 d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
        hydrolysis $t_{1/2}$ ~ 1 yr for trialkyl phosphates (Wolfe 1980);
        $t_{1/2}$ = 58 h in the water containing killifish and more than 100 h for goldfish (Sasaki et al. 1981)
        volatilization $t_{1/2}$ ~ 0.4 d from 1 m deep water (estimated, Muir 1984).
    Groundwater:
    Sediment:
    Soil:
    Biota:

TABLE 15.1.4.3.1.1

Reported aqueous solubilities and vapor pressures of tributyl phosphate 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)	

Aqueous solubility		Vapor pressure					
Higgins et al. 1959		Skene & Krzymien 1995					
shake flask-titration		gas saturation-GC		GC-RT correlation			
t/°C	S/g·m⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				different reference standards			
3.4	1075	0	0.004	170	1042	170	1060
4.0	1012	5	0.01	185	1646	185	1849
5.0	957	15	0.04	200	4442	200	4102
13.0	640	25	0.15	Linear extrapolation eq.*		Linear extrapolation eq.*	
25	422	35	0.39	eq. 1	P/Pa	eq. 1	P/Pa
50	285	50	1.59	A	12.336	A	12.333
		65	7.17	B	4124.2	B	4127.8
		80	31.9				
				170	927	170	993
		eq. 3	P/Pa	185	2179	185	1849
		A	8.85629	200	3030	200	3559
		B	1690.26	Linear extrapolation eq.*		Linear extrapolation eq.*	
		C	–123.431	eq. 1	P/Pa	eq. 1	P/Pa
				A	12.633	A	12.480
				B	4306.7	B	4215.3
				170	1109		
				185	2080		
				200	4408		
				Linear extrapolation eq.*			
				eq. 1	P/Pa		
				A	12.253		
				B	4080.7		

*regression eq. for extrapolation to temp range of gas saturation measurements 0–50°C
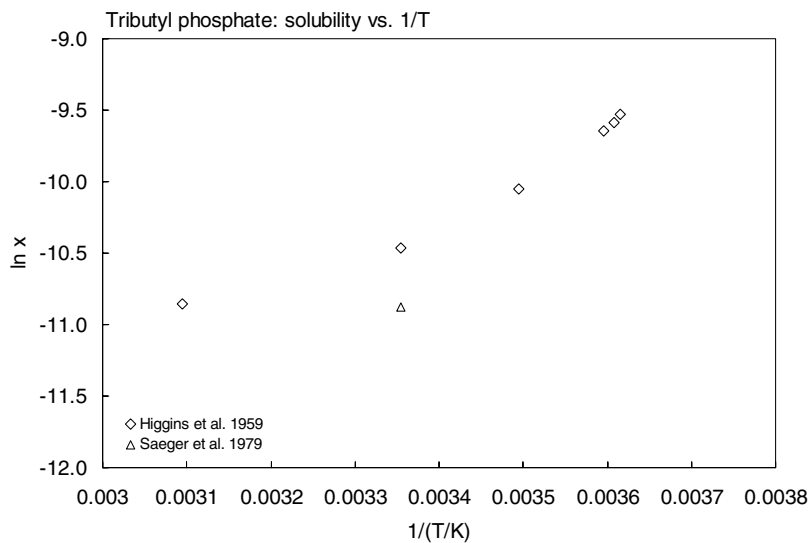
FIGURE 15.1.4.3.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for tributyl phosphate.
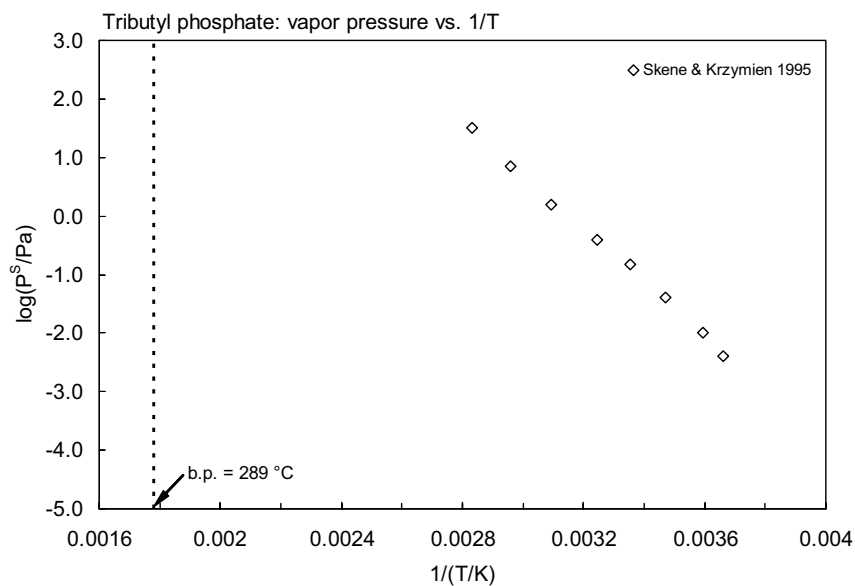
FIGURE 15.1.4.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for tributyl phosphate.

15.1.4.3.2   Tris(2-ethylhexyl) phosphate (TEHP)
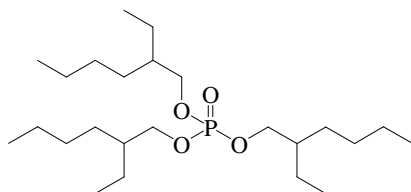
Common Name: Tris(2-ethylhexyl) phosphate
Synonym: TEHP
Chemical Name:
CAS Registry No: 78-42-2
Molecular Formula: $C_{24}H_{51}O_4P$, $(C_8H_{17})_3O_4P$
Molecular Weight: 434.633
Melting Point (°C):
Boiling Point (°C):
   215°C/4 mmHg (Aldrich Catalog 1989–99)
Density (g/cm³ at 20°C): 0.924 (Aldrich catalog 1998–99)
Molar Volume (cm³/mol):
Enthalpy of Vaporization, ΔH_V (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 2 5°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):
   < 1000   (room temp, shake flask-GC, Saeger et al. 1979)
   600   (practical grade, shake flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at 25°C):
   log (P/mmHg) = 12.85 – 5812/(T/K); exptl. data presented in graph and Antoine eq. (effusion, Small et al. 1948)
       (See figure at the end of this section.)
   1.10×10^{-5} (liquid P_L, GC-RT correlation, Hinckley et al. 1990)

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

Octanol/Water Partition Coefficient, log K_{OW}:
   4.23   (shake flask-concn ratio, Saeger et al. 1979)

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

Bioconcentration Factor, log BCF:
   2.40   (calculated, Saeger et al. 1979)

Sorption Partition Coefficient, log K_{OC}:
   3.68   (soil, calculated-K_{OW}, Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
   Volatilization:
   Photolysis:
   Oxidation:
   Hydrolysis:
   Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).
   Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

Groundwater:

Sediment:

Soil:

Biota:
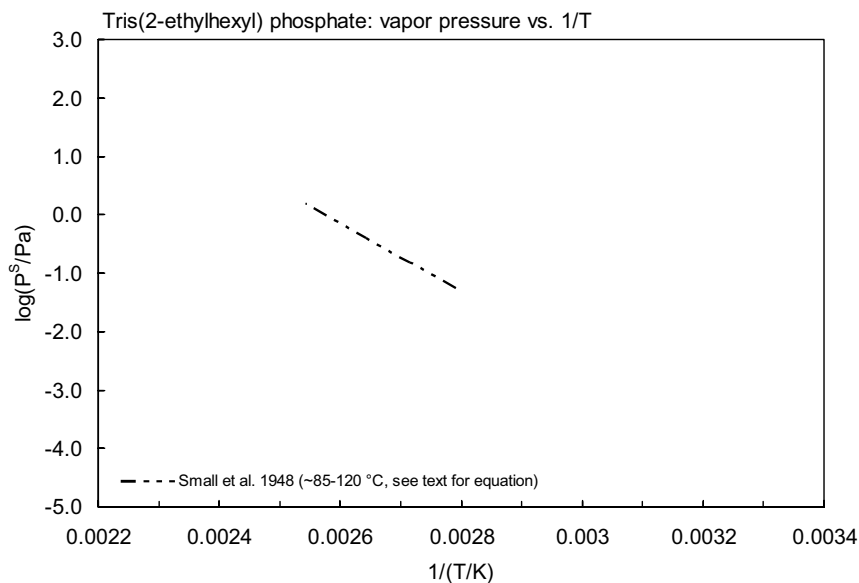
FIGURE 15.1.4.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for *tris*(2-ethylhexyl) phosphate.

15.1.4.4 Trihaloalkyl phosphates

15.1.4.4.1 Tris(2-chloroethyl) phosphate (TCEP)
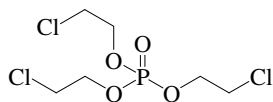
Common Name: Tris(2-chloroethyl) phosphate
Synonym: TCEP
Chemical Name:
CAS Registry No: 115-96-8
Molecular Formula: $C_6H_{12}Cl_3O_4P$, $(C_2H_4Cl)_3O_4P$
Molecular Weight: 285.490
Melting Point (°C): –55
Boiling Point (°C):
    214/25 mmHg (Muir 1984)
    330   (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
    1.390   (Aldrich catalog 1989–99)

Molar Volume (cm³/mol):
    205.4   (20°C, Stephenson & Malanowski 1987)
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):
    7000   (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981)
    7000   (quoted, Muir 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    8.23   (interpolated-Antoine eq., Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 4.346 - 1917/(T/K)$ (Antoine eq., temp range: 293–546 K, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m³/mol at 25°C):
    0.00241   (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, log K_{OW}:
    1.43   (shake flask, Sasaki et al. 1981)
    1.48   (quoted, Muir 1984)

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

Bioconcentration Factor, log BCF:
    2.40   (calculated, Saeger et al. 1979)
    0.34   (killifish, 90-h exposure, static water system, Sasaki et al. 1981)
    – 0.155, –0.046   (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)
    0.36–1.10   (killifish, static water system, Sasaki et al. 1982)
    0.041–1.10   (killifish, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
    2.18   (calculated-K_{OW}, Muir 1984)

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

Volatilization: $t_{1/2} \sim 536$ d from 1 m deep water system (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

biological $t_{1/2} = 1.65$ h and elimination $t_{1/2} = 0.7$ h for killifish (Sasaki et al. 1982).

Half-Lives in the Environment:

Air:

Surface water: first order reduction process in river water, an estimated $t_{1/2} \sim 2.3$ d in Rhine River (Zoeteman et al. 1980);

volatilization $t_{1/2}$(calc) = 536 d from 1 m deep water system (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota: biological $t_{1/2} = 1.65$ h for accumulation, $t_{1/2} = 0.7$ h for elimination in killifish (Sasaki et al. 1982).

15.1.4.4.2   Tris(1,3-dichloropropyl) phosphate (TDCPP)
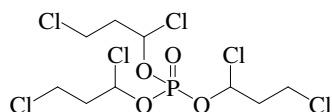
Common Name: Tris(1,3-dichloropropyl) phosphate
Synonym: TDCPP, TCPP, Fyrol FR-2, 1,3-dichloro-2-propanol phosphate (*3:1*), phosphoric acid tris(1,3-dichloro-2-propyl)ester, tris[2-chloro-1-(chloromethyl)ethyl]phosphate
Chemical Name:
Use: flame retardant
CAS Registry No: 40120-74-9
Molecular Formula: $C_9H_{15}Cl_6O_4P$, $(C_3H_5Cl_2)_3O_4P$
Molecular Weight: 430.906
Melting Point (°C):
     26.7   (Muir 1984)
     viscous liquid (Budavari 1989)
Boiling Point (°C):
     236–237/5 mmHg (Muir 1984)
Density (g/cm³ at 20°C):
     1.5022   (Budavari 1989)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.966

Water Solubility (g/m³ or mg/L at 25°C):
     19.2   (Metcalf 1976)
     7.0   (practical grade, shake flask-nephelometry, Hollifield 1979)
     100   (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981, Muir 1984)
     ~ 100   (Budavari 1989)

Vapor Pressure (Pa at 25°C):

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

Octanol/Water Partition Coefficient, log K_{OW}:
     3.76   (shake flask-concn ratio, Sasaki et al. 1981)
     3.74   (quoted, Muir 1984)

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

Bioconcentration Factor, log BCF:
     1.89–2.05   (killifish, 100-h exposure, static system, Sasaki et al. 1981)
     0.48–0.70   (goldfish, 90-h exposure, static system, Sasaki et al. 1981)
     1.67–2.03   (killifish, static system, Sasaki et al. 1982)
     1.49–1.69   (killifish, 32-d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
     3.41   (calculated-K_{OW}, Muir 1984)

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

Hydrolysis:

Biodegradation:

Biotransformation:

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

   $t_{1/2}$ = 31 h in the water containing killifish and $t_{1/2}$ = 42 h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Half-Lives in the Environment:

   Air:

   Surface water: $t_{1/2}$ = 31 h in the water containing killifish and $t_{1/2}$ = 42 h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

   Groundwater:

   Sediment:

   Soil:

   Biota: biological $t_{1/2}$ = 1.65 h (killifish, Sasaki et al. 1982).

15.1.4.4.3   Tris(2,3-dibromopropyl) phosphate (TDBPP)
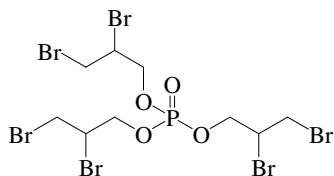
Common Name: Tris(2,3-dibromopropyl) phosphate
Synonym: TDBPP, Tris-BP, 2,3-dibromo-1-propanol phosphate(*3:1*), phosphoric acid tris(2,3-dibromopropyl) ester, Apex 462-3, Flammex AP, Firemaster: V-T 23P, Fyrol HB 32
Chemical Name:
Use: flame retardant
CAS Registry No: 126-72-7
Molecular Formula: $C_9H_{15}Br_6O_4P$, $(C_3H_5Br_2)_3O_4P$
Molecular Weight: 697.610
Melting Point (°C):
    5.5 (Muir 1984)
    viscous liquid (Budavari 1989)
Boiling Point (°C):
    65/0.005 mmHg (Muir 1984)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    8.0   (practical grade, shake flask-nephelometry, Hollifield 1979)
    1.60   (Muir 1984)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):
    0.0108   (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, log K_{OW}:
    4.98   (HPLC-RT correlation, Veith et al. 1979)
    4.39   (Muir 1984)

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

Bioconcentration Factor, log BCF:
    0.44   (calculated-K_{OW}, Veith et al. 1979)

Sorption Partition Coefficient, log K_{OC}:
    3.76   (calculated-K_{OW}, Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
    Volatilization: $t_{1/2}$ (calc) = 1.9 d in 1 m deep water system (Muir 1984).

Half-Lives in the Environment:
    Surface water: volatilization $t_{1/2}$(calc) = 1.9 d in 1 m deep water system (Muir 1984).

TABLE 15.2.1

Summary of physical properties of esters and phthalate esters

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol MW/ρ at 20°C	Le Bas
Aliphatic esters:								
Methyl formate	107-31-3	HCO_2CH_3	60.052	−99	31.7	1	61.64	62.6
Ethyl formate	109-94-4	$HCO_2C_2H_5$	74.079	−79.6	54.4	1	80.35	86.4
Propyl formate	110-74-7	$C_4H_8O_2$	88.106	−92.9	80.9	1	97.30	110.8
Butyl formate	592-84-7	$C_5H_{10}O_2$	102.132	−91.9	106.1	1		133
Isobutyl formate	542-55-2	$C_5H_{10}O_2$	102.132	−95.8	98.2	1		133
Methyl acetate	79-20-9	$(CH_3)_2CO_2$	74.079	−98.25	56.87	1	79.30	84.8
Vinyl acetate	108-05-4	$C_4H_6O_2$	86.09	−93.2	72.8	1	92.40	101.2
Allyl acetate	591-87-7	$C_5H_8O_2$	100.117		103.5	1		125.6
Ethyl acetate	141-78-6	$C_4H_8O_2$	88.106	−83.8	77.11	1	97.83	108.6
Propyl acetate	109-60-4	$C_5H_{10}O_2$	102.132	−93	101.54	1	115.04	133
Butyl acetate	123-86-4	$C_6H_{12}O_2$	116.158	−78	126.1	1	132.54	155.2
Isobutyl acetate	110-19-0	$C_6H_{12}O_2$	116.158	−98.8	116.5	1		155.2
Pentyl acetate	628-63-7	$C_7H_{14}O_2$	130.185	−70.8	149.2	1	148.51	177.4
Isopentyl acetate	123-92-2	$C_7H_{14}O_2$	130.185	−78.5	142.5	1		177.4
Hexyl acetate	142-92-7	$C_8H_{16}O_2$	144.212	−80.9	171.5	1		199.6
Cyclohexyl acetate	622-45-7	$C_8H_{14}O_2$	142.196		173			177.2
2-Ethylhexyl acetate	103-09-3	$C_{10}H_{20}O_2$	172.265	−80	199	1		244
Benzyl acetate	140-11-4	$C_9H_{10}O_2$	150.174	−51.3	213	1		177.2
Ethyl propionate	105-37-3	$C_5H_{10}O_2$	102.132	−73.9	99.1	1		130.8
Ethyl butyrate	105-54-4	$C_6H_{12}O_2$	116.158	−98	121.3	1		153
Methyl acrylate	96-33-3	$C_4H_6O_2$	86.09	< −75	80.7	1	90.29	99.6
Ethyl acrylate	140-88-5	$C_5H_8O_2$	100.117	−71.2	99.4	1	108.42	123.8
Methyl methacrylate	80-62-6	$C_5H_8O_2$	100.117	−47.55	100.5	1	106.06	121.8
Ethyl methacrylate	97-63-2	$C_6H_{10}O_2$	114.142		117			145.6
Aromatic esters:								
Methyl benzoate	93-58-3	$C_8H_8O_2$	136.149	−12.4	199	1	125.07	151.2
Ethyl benzoate	93-89-0	$C_9H_{10}O_2$	150.174	−34	212	1	142.87	175
Propyl benzoate	2315-68-6	$C_{10}H_{12}O_2$	164.201	−51.6	211	1	160.48	199.4
Phenyl benzoate	93-99-2	$C_{13}H_{10}O_2$	198.217	71	314	0.354		221.4
Benzyl benzoate	120-51-4	$C_{14}H_{12}O_2$	212.244	21	323.5	1		243.6

Phthalate esters:

Dimethyl phthalate (DMP)	131-11-3	$C_{10}H_{10}O_4$	194.184	5.5	283.7	1	163.11	206.4
Diethyl phthalate (DEP)	84-66-2	$C_{12}H_{14}O_4$	222.237	–40.5	295	1	198.87	254
Diallyl phthalate (DAP)	131-17-9	$C_{14}H_{14}O_4$	246.259	–77	290		219.68	288
Di-*n*-propyl phthalate (DnPP)	131-16-8	$C_{14}H_{18}O_4$	250.291	–31.0	304.5	1		302.8
Di-isopropyl phthalate (DIPP)	605-45-8	$C_{14}H_{18}O_4$	250.291	liquid		1		302.8
Di-*n*-butyl phthalate (DBP)	84-74-2	$C_{16}H_{22}O_4$	278.344	–35	340	1	265.85	347.2
Di-isobutyl phthalate (DIBP)	84-69-5	$C_{16}H_{22}O_4$	278.344		296.5	1		347.2
Dipentyl phthalate (DPP)	131-18-0	$C_{18}H_{26}O_4$	306.397	< –54.5	342	1		391.6
Dihexyl phthalate (ΔHP)	84-75-3	$C_{20}H_{30}O_4$	334.45	–27.4		1	337.83	436
Butyl 2-ethylhexyl phthalate (BOP)	85-69-8	$C_{20}H_{30}O_4$	334.45	–37		1		436
Di-*n*-octyl phthalate (DOP)	117-84-0	$C_{24}H_{38}O_4$	390.557	25		1	399.34	524.8
Di-isooctyl phthalate (DIOP)	27554-26-3	$C_{24}H_{38}O_4$	390.557		370	1		524.8
bis(2-Ethylhexyl) phthalate (DEHP)	117-81-7	$C_{24}H_{38}O_4$	390.557	–55	384	1	396.79	524.8
Di (hexyl, octyl, decyl) phthalate	39289-94-6	$C_{25}H_{40}O_4$	404.583	–4		1		547.0
Di-isononyl phthalate (DINP)	9727830	$C_{26}H_{42}O_4$	418.609	–48		1	420.71	569.2
Di-isodecyl phthalate (DIDP)	26761-40-0	$C_{28}H_{46}O_4$	446.663	–50		1		613.6
Diundecyl phthalate (DUP)	3648-20-2	$C_{30}H_{50}O_4$	474.716	35.5		0.789		658.0
Ditridecyl phthalate (DTDP)	43617	$C_{34}H_{58}O_4$	530.823	–37		1		746.8
Butyl benzyl phthalate (BBP)	85-68-7	$C_{19}H_{20}O_4$	312.360	–35	370	1		369.2

Phosphate esters:

t-Butylphenyl diphenyl phosphate	56803-37-3	$C_{22}H_{23}O_4P$	382.389	–21		1		
Cresyl diphenyl phosphate (CDP)	26444-49-5	$C_{19}H_{17}O_4P$	340.309					
Isopropylphenyl diphenyl phosphate (IPPDP)	28108-99-8	$C_{21}H_{21}O_4P$	368.362	–26		1		
4-Cumylphenyl diphenyl phosphate	84602-56-2	$C_{27}H_{25}O_4P$	444.458					
Nonylphenyl diphenyl phosphate	13418387	$C_{27}H_{33}O_4P$	452.522					
Triphenyl phosphate (TPP)	115-86-6	$C_{18}H_{15}O_4P$	326.283	50.5		0.562		
Tricresyl phosphate (TCP)	1330-78-5	$C_{21}H_{21}O_4P$	368.362					
Trixylenyl phosphate (TXP)	25155-23-1	$C_{24}H_{27}O_4P$	410.442					
Dibutyl phenyl phosphate (DBPP)	2528-26-1	$C_{14}H_{23}O_4P$	286.303					
2-Ethylhexyl diphenyl phosphate	1241-94-7	$C_{20}H_{27}O_4P$	362.399	–80		1		
Isodecyl diphenyl phosphate (IDDP)	29761-21-5	$C_{22}H_{31}O_4P$	390.452	< –50		1		
Tributylphosphate (TBP)	126-73-8	$C_{12}H_{27}O_4P$	266.314	< –80		1		
Tris(2-ethylhexyl) phosphate	78-42-2	$C_{24}H_{51}O_4P$	434.633					
Tris(2-chloroethyl) phosphate	115-96-8	$C_6H_{12}Cl_3O_4P$	285.49			1		
Tris(1,3-dichloropropyl) phosphate	40120-74-9	$C_9H_{15}Cl_6O_4P$	430.906	26.7		0.962		
Tris(2,3-dibromopropyl) phosphate	126-72-7	$C_9H_{15}Br_6O_4P$	697.61	5.5		1		

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 15.2.2
Summary of selected physical-chemical properties of esters and phthalate esters at 25°C

| Compound | Vapor pressure | | Solubility | | | log K_{OW} | Henry's law constant H/(Pa·m³/mol) | | |
	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)		calcd P/C	exptl (a)	exptl (b)
Aliphatic esters:									
Methyl formate	78060	78060	230000	3830	3830	–0.26	20.38		
Ethyl formate	32370	32600	118000	1593	1593	0.23	20.32		
Propyl formate	11030	11030	20500	232.7	232.7	0.73	47.40		
Butyl formate	3840	3840							
Isobutyl formate	5343	5400	10000	97.91	97.91		54.57		
Methyl acetate	28800	28800	245000	3307	3307	0.23	8.708	0.65	13.06
Vinyl acetate	14100	14100	20000	232.3	232.3	0.73	60.69		
Allyl acetate	6130	6130							
Ethyl acetate	12600	12600	80800	917.1	917.1		13.74		17.2
Propyl acetate	4500	4500	21000	205.6	205.6	1.24	21.88		22.09
Butyl acetate	1600	1600	6000	51.65	51.65	1.82	30.98		29.506
Isobutyl acetate	2860	2860	6300	54.24	54.24	1.6	52.73		
Pentyl acetate	550	550	1700	13.06	13.06	2.42	42.12		35.94
Isopentyl acetate	600	600	2000	15.36	15.36	2.13	39.06		
Hexyl acetate	670	670	500	3.446	3.467		193.2		
2-Ethylhexyl acetate	53	53	98.4	0.5712	0.5712	3.72	92.79		
Phenyl acetate						1.49			
Benzyl acetate	189	189	sl. sol.	sl. sol.		1.96			
Methyl propionate	11600	11600	62370	707.9	707.9		16.39	17.6	
Ethyl propionate	4966	4966	19200	188.0	188.0	1.21	26.42		
Methyl butyrate								20.82	
Ethyl butyrate	2300	2300	6500	55.96	55.96	1.73	41.10		
Methyl pentanoate								32.22	
Methyl hexanoate								37.18	
Methyl octanoate								79.32	
Methyl acrylate	11000	11000	49400	573.8	573.8	0.8	19.17		
Ethyl acrylate	5100	5100	15000	149.82	149.82	1.33	34.041		
Methyl methacrylate	5100	5100	15600	155.8	155.8	1.38	32.73		
Ethyl methacrylate						1.94			

Aromatic esters:							
Methyl benzoate	52.58	52.28	2100	15.42	15.42	2.2	3.389
Ethyl benzoate	24	24	350	2.331	2.331	2.64	10.30
Propyl benzoate	100	100				3.18	
Phenyl benzoate		0.416				3.59	
Benzyl benzoate	0.043	0.043	16	0.0754	0.0754	3.97	0.5704
Phthalate esters:							
Dimethyl phthalate (DMP)	0.22	0.22	4000	20.60	20.60	2.12	0.0107
Diethyl phthalate (DEP)	0.22	0.22	1080	4.859	4.859	2.47	0.0453
Di-n-butyl phthalate (DBP)	0.00187	0.00187	11.2	0.0402	0.0402	4.72	0.0465
Di-n-octyl phthalate (DOP)	1.33×10^{-5}	1.33×10^{-5}	0.0005	1.28×10^{-6}	1.28×10^{-6}	8.06	10.39
bis(2-Ethylhexyl)-phthalate	1.33×10^{-5}	1.33×10^{-5}	0.003	7.68×10^{-6}	7.68×10^{-6}	7.5	1.731
Butyl benzyl phthalate	0.00115	0.00115	2.69	0.0086	0.0086	4.60	0.1335

(a) Buttery et al. 1969

(b) Kieckbusch & King 1979

TABLE 15.2.3
Suggested half-life classes for esters and phthalate esters in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatic esters:				
Methyl formate	3	3	4	5
Ethyl formate	3	3	4	5
Butyl formate	3	3	4	5
Methyl acetate	3	3	4	5
Vinyl acetate	3	3	4	5
Allyl acetate	3	3	4	5
Ethyl acetate	3	3	4	5
Propyl acetate	3	3	4	5
Butyl acetate	3	3	4	5
Pentyl acetate	3	3	4	5
Methyl methacrylate	2	3	4	5
Phthalate esters:				
Dimethyl phthalate (DMP)	4	5	6	7
Diethyl phthalate (DEP)	4	5	6	7
Di-*n*-butyl phthalate (DBP)	3	5	6	7
bis(2-Ethylhexyl)-phthalate (DEHP)	3	5	6	7
Butyl benzyl phthalate (BBP)	3	5	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000
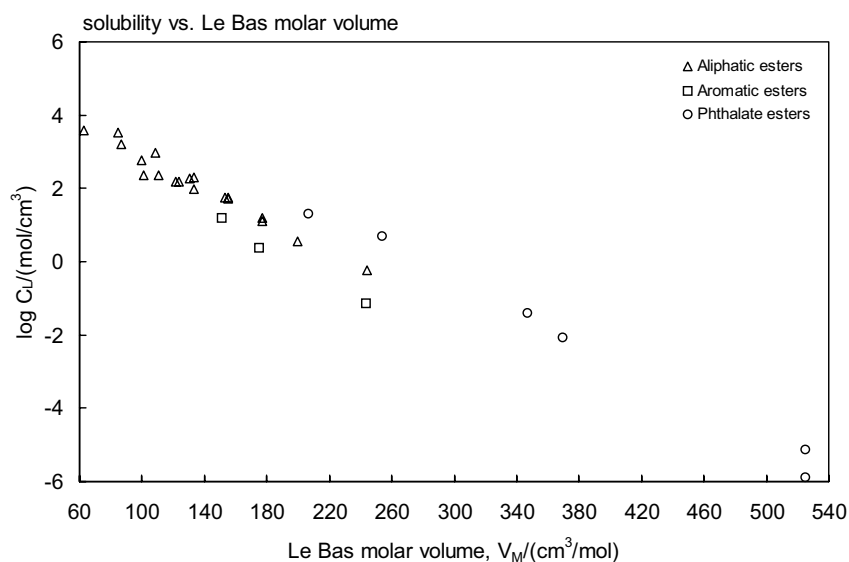
FIGURE 15.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for esters.

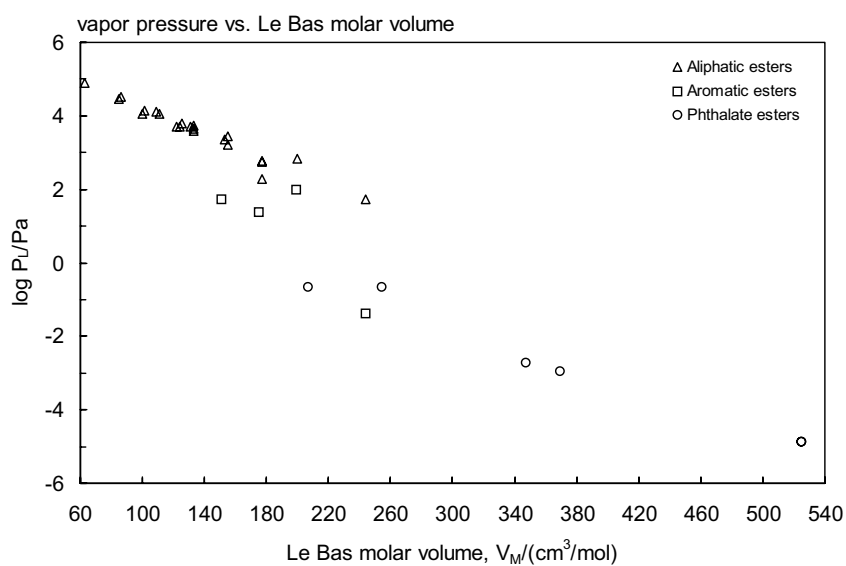**FIGURE 15.2.2** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for esters.
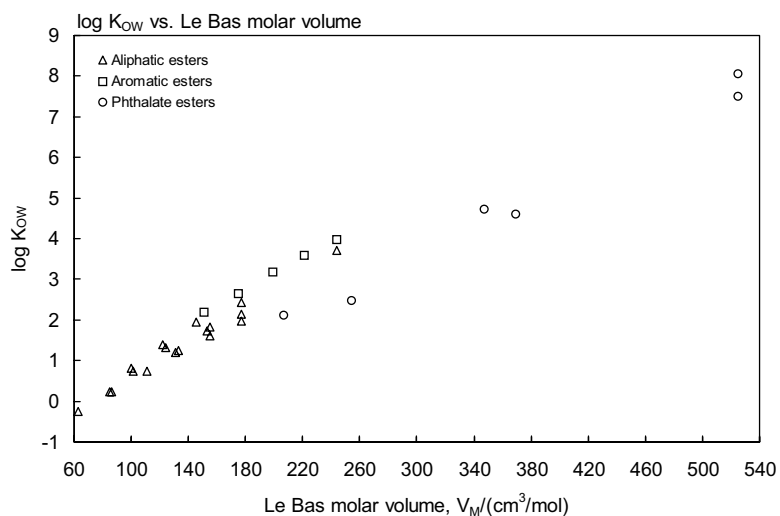
FIGURE 15.2.3 Octanol-water partition coefficient versus Le Bas molar volume for esters.
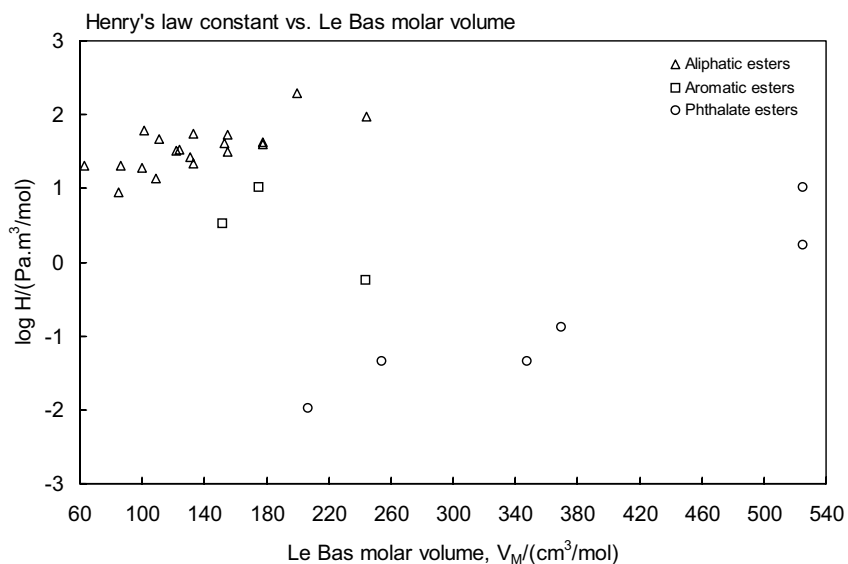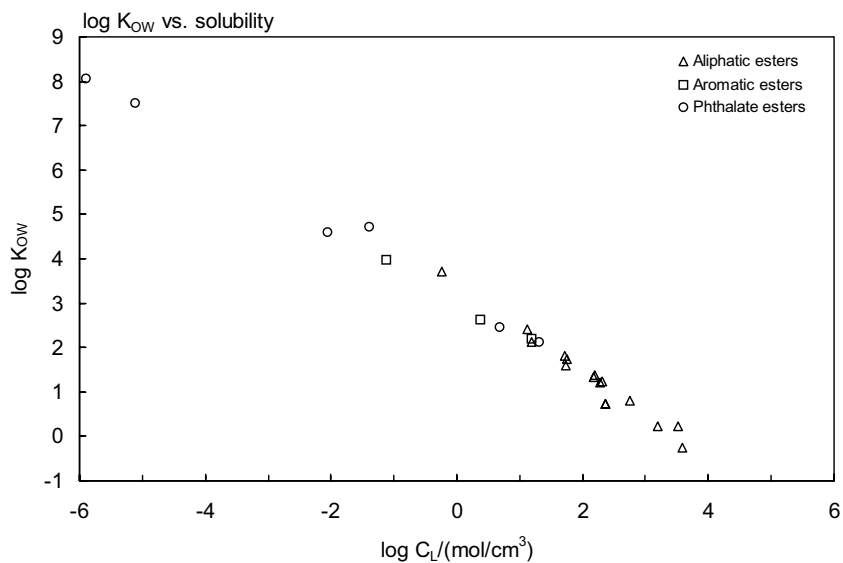

FIGURE 15.2.4 Henry's law constant versus Le Bas molar volume for esters.

FIGURE 15.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for esters.

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