Butanoic acid, methyl ester

Other names:	Butyric acid, methyl ester
	Methyl butanoate
	Methyl butyrate
	Methyl ester of butanoic acid
	Methyl n-butanoate
	Methyl n-butyrate
	NSC 9380
	Propyl butyrate
	UN 1237
	n-Butyric acid methyl ester
	n-C3H7COOCH3
Inchi:	InChI=1S/C5H10O2/c1-3-4-5(6)7-2/h3-4H2,1-2H3
InchiKey:	UUIQMZJEGPQKFD-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CCCC(=O)OC
Mol. weight [g/mol]:	102.13
CAS:	623-42-7

Physical Properties

Property code	Value	Unit	Source
af	0.3800		KDB
affp	836.40	kJ/mol	NIST Webbook
basg	805.40	kJ/mol	NIST Webbook
chl	-2900.00	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	-242.70	kJ/mol	Joback Method
hf	-391.33	kJ/mol	Joback Method
hfus	11.36	kJ/mol	Phase equilibria and the thermodynamic properties of methyl and ethyl esters of carboxylic acids. 1. Methyl n-butanoate and ethyl propanoate
hvap	39.30	kJ/mol	NIST Webbook
hvap	40.60 ± 0.10	kJ/mol	NIST Webbook
hvap	40.60 ± 0.20	kJ/mol	NIST Webbook
hvap	40.30 ± 0.50	kJ/mol	NIST Webbook
hvap	39.30 ± 0.20	kJ/mol	NIST Webbook

hvap	39.28 ± 0.22	kJ/mol	NIST Webbook
hvap	39.80 ± 0.30	kJ/mol	NIST Webbook
hvap	40.10 ± 0.40	kJ/mol	NIST Webbook
hvap	39.33	kJ/mol	NIST Webbook
hvap	39.00 ± 0.40	kJ/mol	NIST Webbook
hvap	40.40	kJ/mol	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.07 ± 0.03	eV	NIST Webbook
log10ws	-0.82		Aqueous Solubility Prediction Method
log10ws	-1.92		Estimated Solubility Method
logp	0.959		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3473.00 ± 81.06	kPa	NIST Webbook
pc	3470.40 ± 40.00	kPa	NIST Webbook
pc	3650.00 ± 202.65	kPa	NIST Webbook
pc	3470.00	kPa	KDB
rhoc	300.27 ± 4.09	kg/m3	NIST Webbook
rhoc	300.17 ± 10.01	kg/m3	NIST Webbook
rhoc	291.08 ± 10.01	kg/m3	NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	720.60		NIST Webbook
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rinpol	706.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	723.00		NIST Webbook
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rinpol	702.00	NIST Webbook
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rinpol	724.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	731.00	NIST Webbook
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rinpol	697.00	NIST Webbook
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rinpol	705.00	NIST Webbook
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ripol	978.00	NIST Webbook
ripol	1001.00	NIST Webbook
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ripol	992.00	NIST Webbook
ripol	982.00	NIST Webbook
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ripol	980.00	NIST Webbook
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ripol	992.00	NIST Webbook
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ripol	1001.00		NIST Webbook
ripol	973.00		NIST Webbook
ripol	995.00		NIST Webbook
ripol	989.00		NIST Webbook
ripol	987.00		NIST Webbook
ripol	982.00		NIST Webbook
ripol	971.00		NIST Webbook
ripol	977.00		NIST Webbook
ripol	994.00		NIST Webbook
tb	375.65 ± 1.00	K	NIST Webbook
tb	369.05 ± 1.00	K	NIST Webbook
tb	369.05 ± 1.00	K	NIST Webbook
tb	376.65 ± 1.00	K	NIST Webbook
tb	375.90	K	KDB
tb	375.53	K	Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane
tb	375.50	K	NIST Webbook
tb	374.00	K	NIST Webbook
tb	375.90	K	NIST Webbook
tb	375.15 ± 2.00	K	NIST Webbook
tb	373.65 ± 1.00	K	NIST Webbook
tb	377.25 ± 1.00	K	NIST Webbook
tb	375.65 ± 1.00	K	NIST Webbook
tb	375.00 ± 2.00	K	NIST Webbook
tb	375.80 ± 1.00	K	NIST Webbook
tb	374.75 ± 1.00	K	NIST Webbook
tb	375.90 ± 1.00	K	NIST Webbook
tb	375.95 ± 1.00	K	NIST Webbook
tb	375.00 ± 2.00	K	NIST Webbook
tb	375.80 ± 0.50	K	NIST Webbook
tb	375.65 ± 1.00	K	NIST Webbook
tb	375.90 ± 1.00	K	NIST Webbook
tb	375.50 ± 1.50	K	NIST Webbook
tb	375.80 ± 0.50	K	NIST Webbook
tc	554.50 ± 1.00	K	NIST Webbook

tc	554.50 ± 1.00	K	NIST Webbook
tc	554.40	K	KDB
tc	544.70 ± 8.00	K	NIST Webbook
tc	551.20 ± 3.00	K	NIST Webbook
tf	187.30	K	KDB
tf	184.55	K	Aqueous Solubility Prediction Method
vc	0.340	m3/kmol	KDB
zc	0.2559460		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.46	J/mol×K	568.66	Joback Method
cpg	180.12	J/mol×K	449.61	Joback Method
cpg	188.08	J/mol×K	479.38	Joback Method
cpg	195.80	J/mol×K	509.14	Joback Method
cpg	203.26	J/mol×K	538.90	Joback Method
cpg	163.46	J/mol×K	390.09	Joback Method
cpg	171.91	J/mol×K	419.85	Joback Method
cpl	198.16	J/mol×K	298.15	NIST Webbook
cpl	200.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0002744	Pa×s	390.09	Joback Method
dvisc	0.0006307	Pa×s	304.18	Joback Method
dvisc	0.0027914	Pa×s	218.27	Joback Method
dvisc	0.0009341	Pa×s	275.54	Joback Method
dvisc	0.0015155	Pa×s	246.91	Joback Method
dvisc	0.0004556	Pa×s	332.82	Joback Method
dvisc	0.0003466	Pa×s	361.45	Joback Method
hvapt	36.40	kJ/mol	366.50	NIST Webbook
hvapt	33.79	kJ/mol	375.90	NIST Webbook
hvapt	36.90	kJ/mol	350.00	NIST Webbook
hvapt	38.40	kJ/mol	338.50	NIST Webbook
hvapt	34.20	kJ/mol	460.00	NIST Webbook
hvapt	42.80	kJ/mol	310.50	NIST Webbook
hvapt	41.10 ± 0.20	kJ/mol	284.00	NIST Webbook
pvap	1.40	kPa	278.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	2.54	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.52	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.47	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.93	kPa	290.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	3.09	kPa	291.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.29	kPa	276.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	3.21	kPa	292.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	3.38	kPa	293.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	3.72	kPa	294.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	4.07	kPa	295.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	4.48	kPa	298.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	5.22	kPa	300.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	5.30	kPa	301.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	5.70	kPa	303.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.10	kPa	285.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.06	kPa	274.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.96	kPa	283.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	1.85	kPa	283.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.71	kPa	281.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.63	kPa	281.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.49	kPa	279.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.24	kPa	285.80	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.94	kPa	291.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
rfi	1.38502		298.15	Excess molar volumes and excess molar enthalpies for binary mixtures of 1,2-dichloropropane with methyl ethanoate, methyl propanoate, and methyl butanoate at T = 298.15K

rfi	1.38600	298.15	Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex and Vex for 25 binary mixtures {xC(u-1)H(2u-1)CO2CH3 + (1-x)alpha,omega-BrCH2(CH2)(v-2)CH2Br}, where u = 1 to 5, alpha = 1 and v = omega = 2 to 6	
rfi	1.38450	298.15	A Study on Alkane + Ester + Ester Systems. Physicochemical Behavior of Binaries and Ternaries of Octane or Iso-octane with Methyl Esters (Ethanoate, Butanoate, Pentanoate)	
rfi	1.37530	318.15	Excess Properties and Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Methyl Esters + tert-Butanol	
rfi	1.38470	298.15	Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Acetonitrile (2) Systems at 93.32 kPa	
rfi	1.38470	298.15	Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Propanenitrile (2) Systems at 93.32 kPa	

rfi	1.38510		298.15	Measurements and Correlations of the Isobaric Vapor Liquid Equilibria of Binary Mixtures and Excess Properties for Mixtures Containing an Alkyl (Methyl, Ethyl) Butanoate with an Alkane (Heptane, Nonane) at 101.3 kPa	
rhol	903.34	kg/m3	288.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhol	806.03	kg/m3	373.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	793.68	kg/m3	383.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	780.99	kg/m3	393.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	

rhol	767.63	kg/m3	403.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	754.74	kg/m3	413.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	741.06	kg/m3	423.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	817.71	kg/m3	363.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	
rhol	897.88	kg/m3	293.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	

rhol	892.38	kg/m3	298.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhol	886.86	kg/m3	303.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhol	881.30	kg/m3	308.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhol	892.62	kg/m3	298.15	Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions	
rhol	870.14	kg/m3	318.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhol	898.00	kg/m3	293.00	KDB	
rhol	829.80	kg/m3	353.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate	

rhol	841.50	kg/m3	343.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate
rhol	853.04	kg/m3	333.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate
rhol	863.41	kg/m3	323.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate
rhol	875.70	kg/m3	313.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate
rhol	886.90	kg/m3	303.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate

rhol	875.74	kg/m3	313.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution
rhol	898.05	kg/m3	293.15	Experimental Investigation of the Thermophysical Properties of the Bio-Aviation Fuel Surrogates: Binary and Ternary Mixtures of n-Dodecane, Methyl Butyrate, and Methyl Decanoate
tcondl	0.13	W/m×K	318.38	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	323.35	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	328.55	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	333.25	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.13	W/m×K	338.40	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	343.25	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	313.29	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	353.35	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	358.18	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	309.31	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	305.42	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.14	W/m×K	301.30	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	298.44	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	297.41	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	293.39	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	288.30	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.15	W/m×K	283.34	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	348.24	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46637e+01
Coeff. B	-3.24931e+03
Coeff. C	-5.15380e+01
Temperature range (K), min.	277.56
Temperature range (K), max.	398.97

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.73784e+01
Coeff. B	-8.00472e+03
Coeff. C	-1.22593e+01
Coeff. D	8.64840e-06
Temperature range (K), min.	187.35
Temperature range (K), max.	554.50

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	898.42
293.15	1000.00	898.68
293.15	3000.00	900.65
293.15	5000.00	902.15
293.15	10000.00	906.55
293.15	15000.00	910.63
293.15	20000.00	914.51
293.15	25000.00	918.33

293.15	30000.00	921.95
293.15	35000.00	925.38
293.15	40000.00	928.67
293.15	50000.00	935.38
293.15	60000.00	941.12
303.15	100.00	886.68
303.15	1000.00	887.75
303.15	3000.00	889.67
303.15	5000.00	891.54
303.15	10000.00	895.99
303.15	15000.00	900.35
303.15	20000.00	904.45
303.15	25000.00	908.4
303.15	30000.00	912.18
303.15	35000.00	915.86
303.15	40000.00	919.34
303.15	50000.00	926.18
303.15	60000.00	932.54
313.15	100.00	875.83
313.15	1000.00	876.3
313.15	3000.00	878.42
313.15	5000.00	880.45
313.15	10000.00	885.34
313.15	15000.00	889.92
313.15	20000.00	894.25
313.15	25000.00	898.53
313.15	30000.00	902.47
313.15	35000.00	906.46
313.15	40000.00	910.02
313.15	50000.00	917.24
313.15	60000.00	923.73
323.15	100.00	864.35
323.15	1000.00	865.42
323.15	3000.00	867.62
323.15	5000.00	869.76
323.15	10000.00	875.02
323.15	15000.00	879.93
323.15	20000.00	884.63
323.15	25000.00	888.92
323.15	30000.00	893.19
323.15	35000.00	897.21
323.15	40000.00	901.15
323.15	50000.00	908.62
323.15	60000.00	915.65

333.15	100.00	853.11
333.15	1000.00	854.08
333.15	3000.00	856.55
333.15	5000.00	858.82
333.15	10000.00	864.28
333.15	15000.00	869.44
333.15	20000.00	874.46
333.15	25000.00	879.2
333.15	30000.00	883.56
333.15	35000.00	887.79
333.15	40000.00	892.1
333.15	50000.00	899.8
333.15	60000.00	906.96
343.15	100.00	841.05
343.15	1000.00	842.4
343.15	3000.00	844.95
343.15	5000.00	847.57
343.15	10000.00	853.35
343.15	15000.00	858.9
343.15	20000.00	864.31
343.15	25000.00	869.1
343.15	30000.00	873.89
343.15	35000.00	878.44
343.15	40000.00	882.65
343.15	50000.00	890.89
343.15	60000.00	898.16
353.15	100.00	829.58
353.15	1000.00	830.8
353.15	3000.00	833.71
353.15	5000.00	836.31
353.15	10000.00	842.65
353.15	15000.00	848.71
353.15	20000.00	854.19
353.15	25000.00	859.51
353.15	30000.00	864.51
353.15	35000.00	869.35
353.15	40000.00	873.76
353.15	50000.00	882.24
353.15	60000.00	890.18
363.15	100.00	817.31
363.15	1000.00	818.87
363.15	3000.00	821.94
363.15	5000.00	824.91
363.15	10000.00	831.48

363.15	15000.00	838.19
363.15	20000.00	843.84
363.15	25000.00	849.26
363.15	30000.00	854.68
363.15	35000.00	859.76
363.15	40000.00	864.61
363.15	50000.00	873.56
363.15	60000.00	881.85

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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility