Butanoic acid, 3-hydroxy-, ethyl ester

Other names:	3-hydroxybutanoic acid ethyl ester
	3-hydroxybutyric acid, ethyl ester
	Butanoic acid, 3-hydroxy-, ethyl ester, (.+/-.)-
	Butyric acid, «beta»-hydroxy-, ethyl ester
	CH3CH(OH)CH2C(O)OC2H5
	DL-3-Hydroxy-n-butyrate ethyl ester
	Ethyl DL-3-hydroxybutyrate
	Ethyl beta-hydroxybutyrate
	Ethyl «beta»-hydroxybutyrate
	Ethyl-dl-beta-hydroxy n-butyrate
	Ethyl-dl-«beta»-hydroxy n-butyrate
	NSC 42916
	NSC 8115
	butyric acid, 3-hydroxy-, ethyl ester
	dl-«beta»-Hydroxy-n-butyric acid ethyl ester
	ethyl .beta.-hydroxybutyrate
	ethyl 3-hydroxybutanoate
	ethyl 3-hydroxybutyrate
Inchi:	InChI=1S/C6H12O3/c1-3-9-6(8)4-5(2)7/h5,7H,3-4H2,1-2H3
InchiKey:	OMSUIQOIVADKIM-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCOC(=O)CC(C)O
Mol. weight [g/mol]:	132.16
CAS:	5405-41-4

Physical Properties

Property code	Value	Unit	Source
gf	-373.54	kJ/mol	Joback Method
hf	-569.48	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	55.90 ± 0.60	kJ/mol	NIST Webbook
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	907.00		NIST Webbook

rinpol	938.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	907.00	NIST Webbook
rinpol	943.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	913.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	908.00	NIST Webbook
rinpol	912.00	NIST Webbook
rinpol	943.00	NIST Webbook
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ripol	1490.00	NIST Webbook

ripol	1524.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	443.20	K	NIST Webbook
tc	679.05	K	Joback Method
tf	275.36	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.76	J/mol×K	504.71	Joback Method
cpg	254.84	J/mol×K	533.77	Joback Method
cpg	263.60	J/mol×K	562.82	Joback Method
cpg	272.02	J/mol×K	591.88	Joback Method
cpg	280.10	J/mol×K	620.94	Joback Method
cpg	287.86	J/mol×K	649.99	Joback Method
cpg	295.29	J/mol×K	679.05	Joback Method
dvisc	0.0210426	Pa×s	275.36	Joback Method
dvisc	0.0055735	Pa×s	313.59	Joback Method
dvisc	0.0019703	Pa×s	351.81	Joback Method
dvisc	0.0008540	Pa×s	390.03	Joback Method
dvisc	0.0004297	Pa×s	428.26	Joback Method
dvisc	0.0002420	Pa×s	466.49	Joback Method
dvisc	0.0001487	Pa×s	504.71	Joback Method
hvapt	55.90	kJ/mol	298.15	Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture:	https://www.doi.org/10.1016/j.tca.2005.03.021
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5405414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume