

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	920.00		NIST Webbook
rinpol	945.00		NIST Webbook

rinpol	945.00	NIST Webbook
rinpol	943.00	NIST Webbook
rinpol	907.00	NIST Webbook
rinpol	943.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	907.00	NIST Webbook
rinpol	912.00	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
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ripol	1522.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1484.00		NIST Webbook
tb	443.20	K	NIST Webbook
tc	679.05	K	Joback Method
tf	275.36	K	Joback Method
vc	0.408	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.29	J/molxK	679.05	Joback Method
cpg	245.76	J/molxK	504.71	Joback Method
cpg	254.84	J/molxK	533.77	Joback Method
cpg	263.60	J/molxK	562.82	Joback Method
cpg	272.02	J/molxK	591.88	Joback Method
cpg	280.10	J/molxK	620.94	Joback Method
cpg	287.86	J/molxK	649.99	Joback Method
dvisc	0.0001487	Paxs	504.71	Joback Method
dvisc	0.0210426	Paxs	275.36	Joback Method
dvisc	0.0055735	Paxs	313.59	Joback Method
dvisc	0.0019703	Paxs	351.81	Joback Method
dvisc	0.0008540	Paxs	390.03	Joback Method
dvisc	0.0004297	Paxs	428.26	Joback Method
dvisc	0.0002420	Paxs	466.49	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

Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture: McGowan Method:

<https://www.doi.org/10.1016/j.tca.2005.03.021>

NIST Webbook:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5405414&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

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

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