Butanoic acid, 2-hydroxy-, ethyl ester

Other names:	Ethyl «alpha»-hydroxybutyrate
	Ethyl 2-hydroxybutanoate
	Ethyl 2-hydroxybutyrate
	2-Hydroxybutyric acid ethyl ester
	Ethyl 2-hydroxybitanoate
Inchi:	InChI=1S/C6H12O3/c1-3-5(7)6(8)9-4-2/h5,7H,3-4H2,1-2H3
InchiKey:	KWWOQRSLYPHAMK-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCOC(=O)C(O)CC
Mol. weight [g/mol]:	132.16
CAS:	52089-54-0

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	54.40	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	910.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	910.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1396.00		NIST Webbook
tb	504.71	K	Joback Method
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	287.86	J/mol×K	649.99	Joback Method
cpg	280.10	J/mol×K	620.94	Joback Method
cpg	272.02	J/mol×K	591.88	Joback Method
cpg	263.60	J/mol×K	562.82	Joback Method
cpg	254.84	J/mol×K	533.77	Joback Method
cpg	295.29	J/mol×K	679.05	Joback Method
dvisc	0.0001487	Pa×s	504.71	Joback Method
dvisc	0.0002420	Pa×s	466.49	Joback Method
dvisc	0.0004297	Pa×s	428.26	Joback Method
dvisc	0.0008540	Pa×s	390.03	Joback Method
dvisc	0.0019703	Pa×s	351.81	Joback Method
dvisc	0.0055735	Pa×s	313.59	Joback Method
dvisc	0.0210426	Pa×s	275.36	Joback Method

Sources

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=C52089540&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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

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