Butanoic acid, 3-hydroxy-

Other names:	Butyric acid, 3-hydroxy- «beta»-Hydroxy-n-butyric acid «beta»-Hydroxybutyric acid 3-Hydroxybutanoic acid 3-Hydroxybutyric acid 3 HBA (.+/-.)-3-Hydroxybutyric acid DL-«beta»-Hydroxybutyric acid NSC 3806
Inchi:	InChI=1S/C4H8O3/c1-3(5)2-4(6)7/h3,5H,2H2,1H3,(H,6,7)
InchiKey:	WHBMMWSBFZVSSR-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	CC(O)CC(=O)O
Mol. weight [g/mol]:	104.10
CAS:	300-85-6

Physical Properties

Property code	Value	Unit	Source
chs	-1787.80	kJ/mol	NIST Webbook
gf	-422.20	kJ/mol	Joback Method
hf	-548.21	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.158		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
rinpol	976.60		NIST Webbook
rinpol	976.60		NIST Webbook
tb	528.71	K	Joback Method
tc	699.49	K	Joback Method
tf	291.41	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.74	J/mol×K	528.71	Joback Method
cpg	188.75	J/mol×K	557.17	Joback Method
cpg	194.50	J/mol×K	585.64	Joback Method
cpg	199.99	J/mol×K	614.10	Joback Method
cpg	205.24	J/mol×K	642.57	Joback Method
cpg	210.24	J/mol×K	671.03	Joback Method
cpg	215.01	J/mol×K	699.49	Joback Method
dvisc	0.0729956	Pa×s	291.41	Joback Method
dvisc	0.0119633	Pa×s	330.96	Joback Method
dvisc	0.0028846	Pa×s	370.51	Joback Method
dvisc	0.0009152	Pa×s	410.06	Joback Method
dvisc	0.0003553	Pa×s	449.61	Joback Method
dvisc	0.0001608	Pa×s	489.16	Joback Method
dvisc	0.0000819	Pa×s	528.71	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=C300856&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume