Butanoic acid, 3-hydroxy-, methyl ester, (S)-

Other names:	Methyl (S)-(+)-3-hydroxybutyrate
	Butanoic acid, 3-hydroxy-, methyl ester, (3S)-
	(+)-(3S)-3-Hydroxybutanoic acid methyl ester
	(S)-3-Hydroxybutanoic acid methyl ester
	(S)-Methyl 3-hydroxybutanoate
	(.+/-.)-3-Hydroxybutyric acid, methyl ester
	methyl (S)-3-hydroxybutyrate
Inchi:	InChI=1S/C5H10O3/c1-4(6)3-5(7)8-2/h4,6H,3H2,1-2H3/t4-/m1/s1
InchiKey:	LDLDJEAVRNAEBW-SCSAIBSYSA-N
Formula:	C5H10O3
SMILES:	COC(=O)CC(C)O
Mol. weight [g/mol]:	118.13
CAS:	53562-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-381.96	kJ/mol	Joback Method
hf	-548.84	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.070		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	481.83	K	Joback Method
tc	657.66	K	Joback Method
tf	264.09	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.80	J/mol×K	481.83	Joback Method
cpg	241.86	J/mol×K	628.35	Joback Method

cpg	235.00	J/mol×K	599.05	Joback Method
cpg	227.87	J/mol×K	569.74	Joback Method
cpg	220.46	J/mol×K	540.44	Joback Method
cpg	212.77	J/mol×K	511.13	Joback Method
cpg	248.43	J/mol×K	657.66	Joback Method
dvisc	0.0001769	Pa×s	481.83	Joback Method
dvisc	0.0002891	Pa×s	445.54	Joback Method
dvisc	0.0005156	Pa×s	409.25	Joback Method
dvisc	0.0010292	Pa×s	372.96	Joback Method
dvisc	0.0023843	Pa×s	336.67	Joback Method
dvisc	0.0067671	Pa×s	300.38	Joback Method
dvisc	0.0255824	Pa×s	264.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.20	K	1.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C53562860&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume