Butanoic acid, 3-hydroxy-3-methyl-, methyl ester

Other names: Butyric acid, 3-hydroxy-3-methyl-, methyl ester
(CH3)2C(OH)CH2C(O)OCH3
Methyl 3-hydroxy-3-methylbutanoate
«beta»-Hydroxyisovaleric acid, methyl ester
Methyl 3-methyl 3-hydroxybutanoate

Inchi: InChI=1S/C6H12O3/c1-6(2,8)4-5(7)9-3/h8H,4H2,1-3H3

InchiKey: JNURPEZKOSMRMZ-UHFFFAOYSA-N

Formula: C6H12O3

SMILES: COC(=O)CC(C)(C)O

Mol. weight [g/mol]: 132.16

CAS: 6149-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-368.26	kJ/mol	Joback Method
hf	-572.95	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	893.60		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	893.60		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1363.00		NIST Webbook
tb	501.92	K	Joback Method
tc	682.72	K	Joback Method
tf	292.78	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	501.92	Joback Method
cpg	258.51	J/mol×K	532.05	Joback Method
cpg	267.61	J/mol×K	562.19	Joback Method
cpg	276.27	J/mol×K	592.32	Joback Method
cpg	284.51	J/mol×K	622.45	Joback Method
cpg	292.32	J/mol×K	652.58	Joback Method
cpg	299.73	J/mol×K	682.72	Joback Method
dvisc	0.0147388	Pa×s	292.78	Joback Method
dvisc	0.0046012	Pa×s	327.64	Joback Method
dvisc	0.0017968	Pa×s	362.49	Joback Method
dvisc	0.0008275	Pa×s	397.35	Joback Method
dvisc	0.0004319	Pa×s	432.21	Joback Method
dvisc	0.0002484	Pa×s	467.06	Joback Method
dvisc	0.0001543	Pa×s	501.92	Joback Method

Sources

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=C6149457&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
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