Methyl L-(+)-«beta»-hydroxyisobutyrate

Other names:	(2R)-3-hydroxy-2-methyl-propanoic acid methyl ester
	(2S)-3-hydroxy-2-methyl-propanoic acid methyl ester
	(S)-(+)-Methyl 3-hydroxy-2-methylpropionate
	Methyl (S)-(+)-3-hydroxy-2-methyl-propionate
Inchi:	InChI=1S/C5H10O3/c1-4(3-6)5(7)8-2/h4,6H,3H2,1-2H3/t4-/m1/s1
InchiKey:	ATCCIZURPPEVIZ-SCSAIBSYSA-N
Formula:	C5H10O3
SMILES:	COC(=O)C(C)CO
Mol. weight [g/mol]:	118.13
CAS:	80657-57-4

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	0.20		Crippen Method
logp	-0.212		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	248.43	J/mol×K	657.66	Joback Method
cpg	204.80	J/mol×K	481.83	Joback Method
cpg	212.77	J/mol×K	511.13	Joback Method
cpg	220.46	J/mol×K	540.44	Joback Method
cpg	227.87	J/mol×K	569.74	Joback Method

cpg	235.00	J/mol×K	599.05	Joback Method
cpg	241.86	J/mol×K	628.35	Joback Method
dvisc	0.0001769	Pa×s	481.83	Joback Method
dvisc	0.0255824	Pa×s	264.09	Joback Method
dvisc	0.0067671	Pa×s	300.38	Joback Method
dvisc	0.0023843	Pa×s	336.67	Joback Method
dvisc	0.0010292	Pa×s	372.96	Joback Method
dvisc	0.0005156	Pa×s	409.25	Joback Method
dvisc	0.0002891	Pa×s	445.54	Joback Method
rhol	1067.50	kg/m3	298.15	Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.019
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=C80657574&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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume