

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/molxK	657.66	Joback Method
cpg	241.86	J/molxK	628.35	Joback Method
cpg	235.00	J/molxK	599.05	Joback Method
cpg	227.87	J/molxK	569.74	Joback Method
cpg	220.46	J/molxK	540.44	Joback Method

cpg	212.77	J/molxK	511.13	Joback Method
cpg	204.80	J/molxK	481.83	Joback Method
dvisc	0.0255824	Paxs	264.09	Joback Method
dvisc	0.0001769	Paxs	481.83	Joback Method
dvisc	0.0002891	Paxs	445.54	Joback Method
dvisc	0.0005156	Paxs	409.25	Joback Method
dvisc	0.0010292	Paxs	372.96	Joback Method
dvisc	0.0023843	Paxs	336.67	Joback Method
dvisc	0.0067671	Paxs	300.38	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:

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>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C80657574&Units=SI>

<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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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