methyl 3-hydroxy-3-methylpentanoate

Inchi: InChI=1S/C7H14O3/c1-4-7(2,9)5-6(8)10-3/h9H,4-5H2,1-3H3
InchiKey: UDWYINMRIFIIGL-UHFFFAOYSA-N
Formula: C7H14O3
SMILES: CCC(C)(O)CC(=O)OC
Mol. weight [g/mol]: 146.18

Physical Properties

Property code	Value	Unit	Source
gf	-359.84	kJ/mol	Joback Method
hf	-593.59	kJ/mol	Joback Method
hfus	13.35	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
ripol	1448.00		NIST Webbook
tb	524.80	K	Joback Method
tc	703.84	K	Joback Method
tf	304.05	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.93	J/mol×K	524.80	Joback Method
cpg	302.45	J/mol×K	554.64	Joback Method
cpg	312.47	J/mol×K	584.48	Joback Method
cpg	322.01	J/mol×K	614.32	Joback Method
cpg	331.07	J/mol×K	644.16	Joback Method
cpg	339.68	J/mol×K	674.00	Joback Method
cpg	347.85	J/mol×K	703.84	Joback Method
dvisc	0.0121392	Pa×s	304.05	Joback Method
dvisc	0.0037644	Pa×s	340.84	Joback Method

dvisc	0.0014665	Pa×s	377.63	Joback Method
dvisc	0.0006754	Pa×s	414.42	Joback Method
dvisc	0.0003530	Pa×s	451.22	Joback Method
dvisc	0.0002034	Pa×s	488.01	Joback Method
dvisc	0.0001267	Pa×s	524.80	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=R335065&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume