

methyl 3-hydroxyisovalerate

Inchi:	InChI=1S/C8H14O4/c1-6(9)12-8(2,3)5-7(10)11-4/h5H2,1-4H3
InchiKey:	OORCPKWHUGCFTN-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	COC(=O)CC(C)(C)OC(C)=O
Mol. weight [g/mol]:	174.19

Physical Properties

Property code	Value	Unit	Source
gf	-448.52	kJ/mol	Joback Method
hf	-706.80	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	50.42	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.891		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
ripol	1642.00		NIST Webbook
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tb	531.79	K	Joback Method
tc	726.31	K	Joback Method
tf	326.66	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.66	J/molxK	531.79	Joback Method
cpg	337.91	J/molxK	564.21	Joback Method
cpg	349.58	J/molxK	596.63	Joback Method
cpg	360.67	J/molxK	629.05	Joback Method
cpg	371.20	J/molxK	661.47	Joback Method
cpg	381.16	J/molxK	693.89	Joback Method
cpg	390.56	J/molxK	726.31	Joback Method
dvisc	0.0023952	Paxs	326.66	Joback Method

dvisc	0.0013252	Paxs	360.85	Joback Method
dvisc	0.0008123	Paxs	395.04	Joback Method
dvisc	0.0005383	Paxs	429.23	Joback Method
dvisc	0.0003790	Paxs	463.41	Joback Method
dvisc	0.0002801	Paxs	497.60	Joback Method
dvisc	0.0002151	Paxs	531.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R332759&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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