3-Hydroxy-3-methylvaleric acid

Other names: 3-Hydroxy-3-methylpentanoic acid
Inchi: InChI=1S/C6H12O3/c1-3-6(2,9)4-5(7)8/h9H,3-4H2,1-2H3,(H,7,8)
InchiKey: KEGHVPSZIWXTPY-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CCC(C)(O)CC(=O)O
Mol. weight [g/mol]: 132.16
CAS: 150-96-9

Physical Properties

Property code	Value	Unit	Source
gf	-400.08	kJ/mol	Joback Method
hf	-592.96	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.622		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
ripol	2288.00		NIST Webbook
ripol	2288.00		NIST Webbook
tb	571.68	K	Joback Method
tc	745.53	K	Joback Method
tf	331.37	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.59	J/mol×K	571.68	Joback Method
cpg	279.74	J/mol×K	600.66	Joback Method
cpg	287.45	J/mol×K	629.63	Joback Method
cpg	294.75	J/mol×K	658.61	Joback Method
cpg	301.65	J/mol×K	687.58	Joback Method
cpg	308.18	J/mol×K	716.56	Joback Method

cpg	314.36	J/mol×K	745.53	Joback Method
dvisc	0.0218901	Pa×s	331.37	Joback Method
dvisc	0.0045887	Pa×s	371.42	Joback Method
dvisc	0.0013039	Pa×s	411.47	Joback Method
dvisc	0.0004632	Pa×s	451.52	Joback Method
dvisc	0.0001947	Pa×s	491.58	Joback Method
dvisc	0.0000933	Pa×s	531.63	Joback Method
dvisc	0.0000496	Pa×s	571.68	Joback Method

Sources

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=C150969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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