3-Hydroxy-3-methylbutanoic acid

Other names: Butyric acid, 3-hydroxy-3-methyl-
«beta»-Hydroxy-isovaleric acid
3-Hydroxyisovaleric acid
3-Hydroxy-3-methylbutanoic acid
Inchi: InChI=1S/C5H10O3/c1-5(2,8)3-4(6)7/h8H,3H2,1-2H3,(H,6,7)
InchiKey: AXFYFNCPONWUHW-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: CC(C)(O)CC(=O)O
Mol. weight [g/mol]: 118.13

Physical Properties

Property code	Value	Unit	Source
hf	-698.17	kJ/mol	Cheméo Relay (1.0)
hfus	11.07	kJ/mol	Joback Method
hvap	78.91	kJ/mol	Cheméo Relay (1.0)
ie	10.31	eV	Cheméo Relay (1.0)
log10ws	0.98		Cheméo Relay (1.0)
logp	0.232		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
rinpol	985.20		NIST Webbook
rinpol	985.20		NIST Webbook
tb	474.45	K	Cheméo Relay (1.0)
tf	378.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.03	J/mol×K	548.80	Joback Method
cpg	235.28	J/mol×K	578.00	Joback Method
cpg	242.14	J/mol×K	607.20	Joback Method
cpg	248.61	J/mol×K	636.41	Joback Method
cpg	254.72	J/mol×K	665.61	Joback Method
cpg	260.49	J/mol×K	694.81	Joback Method
cpg	265.93	J/mol×K	724.01	Joback Method

dvisc	0.0296306	Pa×s	320.10	Joback Method
dvisc	0.0061970	Pa×s	358.22	Joback Method
dvisc	0.0017512	Pa×s	396.33	Joback Method
dvisc	0.0006177	Pa×s	434.45	Joback Method
dvisc	0.0002578	Pa×s	472.57	Joback Method
dvisc	0.0001226	Pa×s	510.68	Joback Method
dvisc	0.0000646	Pa×s	548.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625081&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point