2-Hydroxy-2-methylbutyric acid

Other names: Butanoic acid, 2-hydroxy-2-methyl-
2-Hydroxy-2-methylbutanoic acid
Inchi: InChI=1S/C5H10O3/c1-3-5(2,8)4(6)7/h8H,3H2,1-2H3,(H,6,7)
InchiKey: MBIQENSCDNJOIY-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: CCC(C)(O)C(=O)O
Mol. weight [g/mol]: 118.13
CAS: 3739-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-408.50	kJ/mol	Joback Method
hf	-572.32	kJ/mol	Joback Method
hfus	11.07	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.232		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
tb	548.80	K	Joback Method
tc	724.01	K	Joback Method
tf	320.10	K	Joback Method
vc	0.348	m3/kmol	Joback Method

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

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=C3739308&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume