3-Hydroxy-2-methylbutanenitrile

Inchi: InChI=1S/C5H9NO/c1-4(3-6)5(2)7/h4-5,7H,1-2H3
InchiKey: ISMAITBIVCNVDT-UHFFFAOYSA-N
Formula: C5H9NO
SMILES: CC(O)C(C)C#N
Mol. weight [g/mol]: 99.13
CAS: 38046-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-17.30	kJ/mol	Joback Method
hf	-144.44	kJ/mol	Joback Method
hfus	7.25	kJ/mol	Joback Method
hvap	53.11	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.527		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	911.10		NIST Webbook
rinpol	911.10		NIST Webbook
tb	507.18	K	Joback Method
tc	696.56	K	Joback Method
tf	241.92	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.58	J/mol×K	507.18	Joback Method
cpg	199.01	J/mol×K	538.74	Joback Method
cpg	206.10	J/mol×K	570.31	Joback Method
cpg	212.86	J/mol×K	601.87	Joback Method
cpg	219.29	J/mol×K	633.43	Joback Method
cpg	225.41	J/mol×K	665.00	Joback Method
cpg	231.23	J/mol×K	696.56	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=C38046467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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