

1-Methyl-muco-inositol

Inchi:	InChI=1S/C7H14O6/c1-7(13)5(11)3(9)2(8)4(10)6(7)12/h2-6,8-13H,1H3/t2?,3-,4?,5?,6-,7?
InchiKey:	AJGYLNFUYLRZFR-OCHHZKIDSA-N
Formula:	C7H14O6
SMILES:	CC1(O)C(O)C(O)C(O)C(O)C1O
Mol. weight [g/mol]:	194.18

Physical Properties

Property code	Value	Unit	Source
gf	-832.45	kJ/mol	Joback Method
hf	-1133.33	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	128.98	kJ/mol	Joback Method
log10ws	1.10		Crippen Method
logp	-3.444		Crippen Method
mcvol	133.850	ml/mol	McGowan Method
pc	6369.39	kPa	Joback Method
rinqol	1866.00		NIST Webbook
tb	909.08	K	Joback Method
tc	1115.31	K	Joback Method
tf	543.65	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.30	J/molxK	909.08	Joback Method
cpg	501.52	J/molxK	943.45	Joback Method
cpg	511.66	J/molxK	977.82	Joback Method
cpg	521.79	J/molxK	1012.19	Joback Method
cpg	531.98	J/molxK	1046.57	Joback Method
cpg	542.32	J/molxK	1080.94	Joback Method
cpg	552.86	J/molxK	1115.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R304135&Units=SI

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

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