

1,6-Hexanediol, 3-methyl-

Inchi:	InChI=1S/C7H16O2/c1-7(4-6-9)3-2-5-8/h7-9H,2-6H2,1H3
InchiKey:	SQAJRDHPLTWZQT-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CC(CCO)CCCO
Mol. weight [g/mol]:	132.20
CAS:	4089-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-268.02	kJ/mol	Joback Method
hf	-497.55	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.777		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	543.48	K	Joback Method
tc	703.08	K	Joback Method
tf	275.29	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.37	J/molxK	543.48	Joback Method
cpg	308.91	J/molxK	570.08	Joback Method
cpg	318.08	J/molxK	596.68	Joback Method
cpg	326.88	J/molxK	623.28	Joback Method
cpg	335.33	J/molxK	649.88	Joback Method
cpg	343.43	J/molxK	676.48	Joback Method
cpg	351.20	J/molxK	703.08	Joback Method
dvisc	0.1642467	Paxs	275.29	Joback Method
dvisc	0.0172033	Paxs	319.99	Joback Method

dvisc	0.0031328	Paxs	364.69	Joback Method
dvisc	0.0008275	Paxs	409.38	Joback Method
dvisc	0.0002841	Paxs	454.08	Joback Method
dvisc	0.0001181	Paxs	498.78	Joback Method
dvisc	0.0000567	Paxs	543.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4089718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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