

1,2-Hexanediol, 2-methyl-

Inchi:	InChI=1S/C7H16O2/c1-3-4-5-7(2,9)6-8/h8-9H,3-6H2,1-2H3
InchiKey:	BSJQMNIJQVVJPX-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCCC(C)(O)CO
Mol. weight [g/mol]:	132.20
CAS:	56255-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-262.74	kJ/mol	Joback Method
hf	-501.02	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.920		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	540.69	K	Joback Method
tc	705.20	K	Joback Method
tf	292.71	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.55	J/molxK	540.69	Joback Method
cpg	312.41	J/molxK	568.11	Joback Method
cpg	321.81	J/molxK	595.53	Joback Method
cpg	330.76	J/molxK	622.94	Joback Method
cpg	339.28	J/molxK	650.36	Joback Method
cpg	347.40	J/molxK	677.78	Joback Method
cpg	355.13	J/molxK	705.20	Joback Method
dvisc	0.0841554	Paxs	292.71	Joback Method
dvisc	0.0117921	Paxs	334.04	Joback Method

dvisc	0.0025471	Paxs	375.37	Joback Method
dvisc	0.0007456	Paxs	416.70	Joback Method
dvisc	0.0002724	Paxs	458.03	Joback Method
dvisc	0.0001176	Paxs	499.36	Joback Method
dvisc	0.0000577	Paxs	540.69	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=C56255506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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