

2,11-Dimethyl-2,11-dodecanediol

Inchi:	InChI=1S/C14H30O2/c1-13(2,15)11-9-7-5-6-8-10-12-14(3,4)16/h15-16H,5-12H2,1-4H3
InchiKey:	KKADLXHVRDQAFN-UHFFFAOYSA-N
Formula:	C14H30O2
SMILES:	CC(C)(O)CCCCCCCCC(C)(C)O
Mol. weight [g/mol]:	230.39
CAS:	22092-59-7

Physical Properties

Property code	Value	Unit	Source
chs	-8950.00 ± 4.00	kJ/mol	NIST Webbook
gf	-200.96	kJ/mol	Joback Method
hf	-654.25	kJ/mol	Joback Method
hfs	-846.00 ± 4.00	kJ/mol	NIST Webbook
hfus	25.36	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.649		Crippen Method
mcvol	219.860	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
tb	697.62	K	Joback Method
tc	867.72	K	Joback Method
tf	374.02	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.66	J/mol×K	697.62	Joback Method
cpg	672.17	J/mol×K	725.97	Joback Method
cpg	685.97	J/mol×K	754.32	Joback Method
cpg	699.09	J/mol×K	782.67	Joback Method
cpg	711.58	J/mol×K	811.02	Joback Method
cpg	723.48	J/mol×K	839.37	Joback Method
cpg	734.83	J/mol×K	867.72	Joback Method

dvisc	0.0074894	Pa×s	374.02	Joback Method
dvisc	0.0011546	Pa×s	427.95	Joback Method
dvisc	0.0002705	Pa×s	481.89	Joback Method
dvisc	0.0000849	Pa×s	535.82	Joback Method
dvisc	0.0000329	Pa×s	589.75	Joback Method
dvisc	0.0000150	Pa×s	643.69	Joback Method
dvisc	0.0000077	Pa×s	697.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22092597&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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