

8-«alpha»-11-Elemodiol

Inchi:	InChI=1S/C14H24O2/c1-6-10-7-13(15)12(14(4,5)16)8-11(10)9(2)3/h6,10-13,15-16H,1-2,
InchiKey:	QKVCTWTVHSDDGI-HNGCFSAESA-N
Formula:	C14H24O2
SMILES:	C=CC1CC(O)C(C(C)(C)O)CC1C(=C)C
Mol. weight [g/mol]:	224.34
CAS:	64373-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-35.35	kJ/mol	Joback Method
hf	-411.13	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	77.06	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.523		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1748.00		NIST Webbook
tb	699.63	K	Joback Method
tc	887.69	K	Joback Method
tf	348.78	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.92	J/molxK	699.63	Joback Method
cpg	624.07	J/molxK	730.97	Joback Method
cpg	639.28	J/molxK	762.32	Joback Method
cpg	653.59	J/molxK	793.66	Joback Method
cpg	667.04	J/molxK	825.01	Joback Method

cpg	679.68	J/mol×K	856.35	Joback Method
cpg	691.53	J/mol×K	887.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64373815&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvac:	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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