9-Hydroxynerolidol

Inchi: InChI=1S/C15H26O2/c1-6-15(5,17)9-7-8-13(4)11-14(16)10-12(2)3/h6,8,10,14,16-17H,1,7

InchiKey: TZCKNDPYYKEPHO-MDWZMJQESA-N

Formula: C15H26O2

SMILES: C=CC(C)(O)CCC=C(C)CC(O)C=C(C)C

Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	33.36	kJ/mol	Joback Method
hf	-331.13	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.367		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1703.00		NIST Webbook
ripol	2560.00		NIST Webbook
tb	728.05	K	Joback Method
tc	908.64	K	Joback Method
tf	328.03	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.10	J/mol×K	728.05	Joback Method
cpg	652.66	J/mol×K	758.15	Joback Method
cpg	665.54	J/mol×K	788.25	Joback Method
cpg	677.81	J/mol×K	818.34	Joback Method
cpg	689.53	J/mol×K	848.44	Joback Method
cpg	700.75	J/mol×K	878.54	Joback Method
cpg	711.55	J/mol×K	908.64	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=R432354&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume