6,7-dihydronerolidol

Inchi: InChI=1S/C15H28O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6,9,14,16H,1,7-8,10-12H
InchiKey: NZWVRMHQZPQHLI-UHFFFAOYSA-N
Formula: C15H28O
SMILES: C=CC(C)(O)CCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	98.51	kJ/mol	Joback Method
hf	-286.33	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.476		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1587.00		NIST Webbook
tb	631.83	K	Joback Method
tc	807.60	K	Joback Method
tf	286.25	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.68	J/mol×K	631.83	Joback Method
cpg	613.05	J/mol×K	661.12	Joback Method
cpg	628.59	J/mol×K	690.42	Joback Method
cpg	643.36	J/mol×K	719.71	Joback Method
cpg	657.39	J/mol×K	749.01	Joback Method
cpg	670.74	J/mol×K	778.30	Joback Method
cpg	683.45	J/mol×K	807.60	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=R300826&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume