Nerolidol oxide

Inchi: InChI=1S/C15H26O/c1-6-14(4)11-8-12-15(5,16-14)10-7-9-13(2)3/h6,9H,1,7-8,10-12H2,2
InchiKey: UCUXXGXEGCFWQD-UHFFFAOYSA-N
Formula: C15H26O
SMILES: C=CC1(C)CCCC(C)(CCC=C(C)C)O1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	154.57	kJ/mol	Joback Method
hf	-187.61	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.637		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	585.63	K	Joback Method
tc	800.10	K	Joback Method
tf	315.52	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.71	J/mol×K	585.63	Joback Method
cpg	566.97	J/mol×K	621.37	Joback Method
cpg	587.00	J/mol×K	657.12	Joback Method
cpg	606.02	J/mol×K	692.86	Joback Method
cpg	624.24	J/mol×K	728.61	Joback Method
cpg	641.90	J/mol×K	764.35	Joback Method

cpg	659.20	J/mol×K	800.10	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=R441833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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