Nerolidol isomer

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

Physical Properties

Property code	Value	Unit	Source
gf	172.62	kJ/mol	Joback Method
hf	-173.62	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.396		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	1551.00		NIST Webbook
rinpol	1550.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2044.00		NIST Webbook
tb	636.31	K	Joback Method
tc	817.59	K	Joback Method
tf	282.21	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.19	J/mol×K	636.31	Joback Method
cpg	591.00	J/mol×K	666.52	Joback Method
cpg	605.97	J/mol×K	696.74	Joback Method
cpg	620.16	J/mol×K	726.95	Joback Method
cpg	633.63	J/mol×K	757.17	Joback Method
cpg	646.44	J/mol×K	787.38	Joback Method

cpg	658.66	J/mol×K	817.59	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=R228081&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