Nerolidyl ethanol

Inchi: InChI=1S/C17H30O/c1-6-17(5,13-14-18)12-8-11-16(4)10-7-9-15(2)3/h6,9,11,18H,1,7-8,1
InchiKey: CGYUIWUXBXZGIW-LFIBNONCSA-N
Formula: C17H30O
SMILES: C=CC(C)(CCO)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 250.42

Physical Properties

Property code	Value	Unit	Source
gf	189.46	kJ/mol	Joback Method
hf	-214.90	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.034		Crippen Method
mcvol	243.360	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook
ripol	2462.00		NIST Webbook
ripol	2462.00		NIST Webbook
tb	682.07	K	Joback Method
tc	861.54	K	Joback Method
tf	304.75	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.52	J/mol×K	682.07	Joback Method
cpg	700.12	J/mol×K	711.98	Joback Method
cpg	715.89	J/mol×K	741.89	Joback Method
cpg	730.88	J/mol×K	771.81	Joback Method
cpg	745.15	J/mol×K	801.72	Joback Method
cpg	758.78	J/mol×K	831.63	Joback Method

cpg	771.82	J/mol×K	861.54	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=R410092&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