nerylacetol [6,10-dimethyl-(Z)-5,9-undecadien-2-ol]

Inchi: InChI=1S/C14H26O/c1-11(2)7-6-8-12(3)13(4)9-10-14(5)15/h7,14-15H,6,8-10H2,1-5H3/b

InchiKey: JWAKIRUDIWHFGT-SEYXRHQNSA-N

Formula: C14H26O

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

Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
gf	62.53	kJ/mol	Joback Method
hf	-284.73	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.230		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
ripol	1930.00		NIST Webbook
ripol	1930.00		NIST Webbook
tb	619.42	K	Joback Method
tc	796.54	K	Joback Method
tf	241.32	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.92	J/mol×K	619.42	Joback Method
cpg	557.66	J/mol×K	648.94	Joback Method
cpg	572.66	J/mol×K	678.46	Joback Method
cpg	586.95	J/mol×K	707.98	Joback Method
cpg	600.57	J/mol×K	737.50	Joback Method
cpg	613.56	J/mol×K	767.02	Joback Method
cpg	625.97	J/mol×K	796.54	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=R327336&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume