cis-Linalool oxide, carbamate

Inchi: InChI=1S/C11H19NO3/c1-5-11(4)7-6-8(14-11)10(2,3)15-9(12)13/h5,8H,1,6-7H2,2-4H3,(H
InchiKey: FMWFOHCSIFNDTM-LDYMZIIASA-N
Formula: C11H19NO3
SMILES: C=CC1(C)CCC(C(C)(C)OC(N)=O)O1
Mol. weight [g/mol]: 213.27

Physical Properties

Property code	Value	Unit	Source
gf	-97.82	kJ/mol	Joback Method
hf	-441.32	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.984		Crippen Method
mcvol	173.980	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	631.15	K	Joback Method
tc	857.37	K	Joback Method
tf	426.94	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.03	J/mol×K	631.15	Joback Method
cpg	500.72	J/mol×K	668.85	Joback Method
cpg	516.40	J/mol×K	706.56	Joback Method
cpg	531.21	J/mol×K	744.26	Joback Method
cpg	545.29	J/mol×K	781.96	Joback Method
cpg	558.81	J/mol×K	819.66	Joback Method
cpg	571.89	J/mol×K	857.37	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=R579438&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