cis-4-hydroxylinalool 3,6 oxide

Inchi: InChI=1S/C10H16O2/c1-5-10(4)9(11)6-8(12-10)7(2)3/h5,9,11H,1,6H2,2-4H3/t9-,10-/m1/s
InchiKey: BMSMUURKSKTZQD-NXEZZACHSA-N
Formula: C10H16O2
SMILES: C=CC1(C)OC(=C(C)C)CC1O
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-41.52	kJ/mol	Joback Method
hf	-286.91	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	58.04	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.006		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
ripol	2057.00		NIST Webbook
ripol	2057.00		NIST Webbook
tb	561.38	K	Joback Method
tc	760.09	K	Joback Method
tf	315.05	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.15	J/mol×K	561.38	Joback Method
cpg	374.79	J/mol×K	594.50	Joback Method
cpg	387.65	J/mol×K	627.62	Joback Method
cpg	399.83	J/mol×K	660.73	Joback Method
cpg	411.43	J/mol×K	693.85	Joback Method
cpg	422.54	J/mol×K	726.97	Joback Method
cpg	433.26	J/mol×K	760.09	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=R401924&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