cis-Dehydroxylinalool oxide

Inchi: InChI=1S/C10H16O/c1-5-10(4)7-6-9(11-10)8(2)3/h5,9H,1-2,6-7H2,3-4H3/t9-,10-/m0/s1
InchiKey: XIGFNCYVSHOLIF-UWVGGRQHSA-N
Formula: C10H16O
SMILES: C=CC1(C)CCC(C(=C)C)O1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	137.68	kJ/mol	Joback Method
hf	-85.28	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	999.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	999.00		NIST Webbook
tb	459.24	K	Joback Method
tc	668.90	K	Joback Method
tf	242.11	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.19	J/mol×K	459.24	Joback Method
cpg	317.88	J/mol×K	494.18	Joback Method
cpg	334.36	J/mol×K	529.13	Joback Method
cpg	349.72	J/mol×K	564.07	Joback Method
cpg	364.10	J/mol×K	599.02	Joback Method
cpg	377.60	J/mol×K	633.96	Joback Method
cpg	390.34	J/mol×K	668.90	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=R626841&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