1,2-Epoxylinalool

Inchi: InChI=1S/C10H18O2/c1-8(2)5-4-6-10(3,11)9-7-12-9/h5,9,11H,4,6-7H2,1-3H3
InchiKey: BXOURKNXQXLKRK-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)=CCCC(C)(O)C1CO1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-54.36	kJ/mol	Joback Method
hf	-362.48	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.883		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
tb	554.88	K	Joback Method
tc	743.23	K	Joback Method
tf	291.17	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.69	J/mol×K	554.88	Joback Method
cpg	396.66	J/mol×K	586.27	Joback Method
cpg	409.78	J/mol×K	617.66	Joback Method
cpg	422.09	J/mol×K	649.05	Joback Method
cpg	433.67	J/mol×K	680.45	Joback Method
cpg	444.58	J/mol×K	711.84	Joback Method
cpg	454.87	J/mol×K	743.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614541&Units=SI
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

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