Linallol oxide isomer # 1

Inchi: InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3
InchiKey: BRHDDEIRQPDPMG-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=CC1(C)CCC(C(C)(C)O)O1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-75.59	kJ/mol	Joback Method
hf	-361.90	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
ripol	1443.00		NIST Webbook
ripol	1443.00		NIST Webbook
tb	551.63	K	Joback Method
tc	752.27	K	Joback Method
tf	321.07	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.75	J/mol×K	551.63	Joback Method
cpg	399.17	J/mol×K	585.07	Joback Method
cpg	413.59	J/mol×K	618.51	Joback Method
cpg	427.13	J/mol×K	651.95	Joback Method
cpg	439.91	J/mol×K	685.39	Joback Method
cpg	452.03	J/mol×K	718.83	Joback Method
cpg	463.60	J/mol×K	752.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610410&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

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