Linalool oxide #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	1437.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1436.00		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

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=R492970&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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