

Linalool oxide, dihydro

Inchi:	InChI=1S/C10H20O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h8,11H,5-7H2,1-4H3
InchiKey:	ZSIHHIBGUWREKL-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCC1(C)CCC(C(C)(C)O)O1
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-163.43	kJ/mol	Joback Method
hf	-487.33	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.105		Crippen Method
mcvol	152.640	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1112.00		NIST Webbook
tb	554.95	K	Joback Method
tc	751.67	K	Joback Method
tf	322.83	K	Joback Method
vc	0.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.51	J/mol×K	554.95	Joback Method
cpg	419.49	J/mol×K	587.74	Joback Method
cpg	434.51	J/mol×K	620.52	Joback Method
cpg	448.66	J/mol×K	653.31	Joback Method
cpg	462.05	J/mol×K	686.09	Joback Method
cpg	474.80	J/mol×K	718.88	Joback Method
cpg	486.99	J/mol×K	751.67	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=R589163&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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