

Anhydrolinalool oxide

Other names:	cis-Dehydroxy linalool oxide Z-Dehydroxy linalool oxide cis-Anhydrolinalool (Z)-anhydrolinalool oxide B
Inchi:	InChI=1S/C10H16O/c1-5-10(4)7-6-9(11-10)8(2)3/h5,9H,1-2,6-7H2,3-4H3
InchiKey:	XIGFNCYVSHOLIF-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	<chem>C=CC1(C)CCC(C(=C)C)O1</chem>
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	1019.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1008.90		NIST Webbook
rinpol	979.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1237.00		NIST Webbook
tb	459.24	K	Joback Method

tc	668.90	K	Joback Method
tf	242.11	K	Joback Method
vc	0.517	m ³ /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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54750695&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
rinpol:	Non-polar retention indices

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

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