

dehydrolinalool oxide

Inchi:	InChI=1S/C10H16O/c1-5-10(4)8-6-7-9(2,3)11-10/h5-7H,1,8H2,2-4H3
InchiKey:	XFDJWESOIHLOCV-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=CC1(C)CC=CC(C)(C)O1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	70.76	kJ/mol	Joback Method
hf	-134.06	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	39.80	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mvol	138.170	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
ripol	1460.00		NIST Webbook
tb	466.35	K	Joback Method
tc	686.95	K	Joback Method
tf	278.97	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.34	J/mol×K	466.35	Joback Method
cpg	320.29	J/mol×K	503.12	Joback Method
cpg	336.75	J/mol×K	539.88	Joback Method
cpg	351.92	J/mol×K	576.65	Joback Method
cpg	366.02	J/mol×K	613.42	Joback Method
cpg	379.23	J/mol×K	650.19	Joback Method
cpg	391.79	J/mol×K	686.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R318931&Units=SI
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

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
mccvol:	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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