

Linalool, methyl ether

Inchi:	InChI=1S/C11H20O/c1-6-11(4,12-5)9-7-8-10(2)3/h6,8H,1,7,9H2,2-5H3
InchiKey:	BARWQAWUANUTNS-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	<chem>C=CC(C)(CCC=C(C)C)OC</chem>
Mol. weight [g/mol]:	168.28

Physical Properties

Property code	Value	Unit	Source
gf	99.09	kJ/mol	Joback Method
hf	-178.48	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	40.56	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.324		Crippen Method
mvol	163.120	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
tb	470.99	K	Joback Method
tc	656.94	K	Joback Method
tf	217.58	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.62	J/mol×K	470.99	Joback Method
cpg	373.09	J/mol×K	501.98	Joback Method
cpg	388.73	J/mol×K	532.97	Joback Method
cpg	403.55	J/mol×K	563.96	Joback Method
cpg	417.61	J/mol×K	594.95	Joback Method
cpg	430.94	J/mol×K	625.94	Joback Method
cpg	443.57	J/mol×K	656.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352636&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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