1,6-Octadien-3-ol, 3,7-dimethyl-, formate

Other names:	Linalool, formate
	Linalyl formate
	Linolool, formate
	3,7-Dimethyl-1,6-octadien-3-ol formate
Inchi:	InChI=1S/C11H18O2/c1-5-11(4,13-9-12)8-6-7-10(2)3/h5,7,9H,1,6,8H2,2-4H3
InchiKey:	JZOCDHMHLGUPFI-UHFFFAOYSA-N
Formula:	C11H18O2
SMILES:	C=CC(C)(CCC=C(C)C)OC=O
Mol. weight [g/mol]:	182.26
CAS:	115-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-0.43	kJ/mol	Joback Method
hf	-264.06	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	47.28	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.850		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1215.40		NIST Webbook
rinpol	1215.40		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1201.70		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1206.00		NIST Webbook

rinpol	1206.00		NIST Webbook
rinpol	1201.70		NIST Webbook
rinpol	1215.40		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1256.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	519.65	K	Joback Method
tc	710.46	K	Joback Method
tf	259.58	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.84	J/mol×K	519.65	Joback Method
cpg	396.77	J/mol×K	551.45	Joback Method
cpg	410.87	J/mol×K	583.25	Joback Method
cpg	424.20	J/mol×K	615.06	Joback Method
cpg	436.79	J/mol×K	646.86	Joback Method
cpg	448.67	J/mol×K	678.66	Joback Method
cpg	459.90	J/mol×K	710.46	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115991&Units=SI

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

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