Dihydrolinalyl acetate

Other names: 6,7-Dihydrolinalyl acetate
Inchi: InChI=1S/C12H22O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6,10H,1,7-9H2,2-5H3
InchiKey: DMSMQGBPJBKXNU-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CC(C)(CCCC(C)C)OC(C)=O
Mol. weight [g/mol]: 198.30
CAS: 108597-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-95.52	kJ/mol	Joback Method
hf	-424.41	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	49.11	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.320		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	543.26	K	Joback Method
tc	728.86	K	Joback Method
tf	282.82	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.59	J/mol×K	543.26	Joback Method
cpg	464.05	J/mol×K	574.19	Joback Method
cpg	479.68	J/mol×K	605.13	Joback Method
cpg	494.53	J/mol×K	636.06	Joback Method
cpg	508.61	J/mol×K	666.99	Joback Method
cpg	521.96	J/mol×K	697.93	Joback Method
cpg	534.60	J/mol×K	728.86	Joback Method
dvisc	0.0051988	Pa×s	282.82	Joback Method
dvisc	0.0020082	Pa×s	326.23	Joback Method
dvisc	0.0009699	Pa×s	369.63	Joback Method
dvisc	0.0005458	Pa×s	413.04	Joback Method
dvisc	0.0003427	Pa×s	456.45	Joback Method
dvisc	0.0002333	Pa×s	499.85	Joback Method
dvisc	0.0001688	Pa×s	543.26	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108597906&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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