Dihydrolinalool acetate

Inchi: InChI=1S/C12H22O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h8H,6-7,9H2,1-5H3
InchiKey: WLAIKFKCSAXVJL-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCC(C)(CCC=C(C)C)OC(C)=O
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-109.25	kJ/mol	Joback Method
hf	-437.13	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.465		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1262.00		NIST Webbook
tb	551.06	K	Joback Method
tc	740.34	K	Joback Method
tf	280.54	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.55	J/mol×K	551.06	Joback Method
cpg	465.02	J/mol×K	582.61	Joback Method
cpg	480.64	J/mol×K	614.15	Joback Method
cpg	495.44	J/mol×K	645.70	Joback Method
cpg	509.47	J/mol×K	677.24	Joback Method

cpg	522.75	J/mol×K	708.79	Joback Method
cpg	535.33	J/mol×K	740.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203260&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume