Dihydromyrcenyl acetate

Other names: 2-methyl-6-methylene-2-octyl acetate
Inchi: InChI=1S/C12H22O2/c1-5-10(2)7-6-8-11(3)9-14-12(4)13/h11H,2,5-9H2,1,3-4H3
InchiKey: IRRIQZAIMANVTH-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=C(CC)CCCC(C)COC(C)=O
Mol. weight [g/mol]: 198.30
CAS: 88969-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-106.91	kJ/mol	Joback Method
hf	-425.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1202.00		NIST Webbook
ripol	1431.00		NIST Webbook
tb	546.37	K	Joback Method
tc	725.06	K	Joback Method
tf	266.44	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.43	J/mol×K	546.37	Joback Method
cpg	460.15	J/mol×K	576.15	Joback Method
cpg	475.20	J/mol×K	605.93	Joback Method
cpg	489.59	J/mol×K	635.71	Joback Method

cpg	503.34	J/mol×K	665.50	Joback Method
cpg	516.46	J/mol×K	695.28	Joback Method
cpg	528.96	J/mol×K	725.06	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=C88969419&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume