dihydrogeranyl acetate

Inchi: InChI=1S/C12H22O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h8,10H,5-7,9H2,1-4H3/b11-8+
InchiKey: LZLOAANJNAQPIH-DHZHZOJOSA-N
Formula: C12H22O2
SMILES: CC(=O)OCC=C(C)CCCC(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-114.53	kJ/mol	Joback Method
hf	-433.66	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1332.20		NIST Webbook
rinpol	1332.20		NIST Webbook
tb	553.85	K	Joback Method
tc	736.57	K	Joback Method
tf	263.12	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.83	J/mol×K	553.85	Joback Method
cpg	461.72	J/mol×K	584.30	Joback Method
cpg	476.90	J/mol×K	614.76	Joback Method
cpg	491.38	J/mol×K	645.21	Joback Method
cpg	505.19	J/mol×K	675.66	Joback Method
cpg	518.34	J/mol×K	706.11	Joback Method
cpg	530.86	J/mol×K	736.57	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=R185434&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