«gamma»-isogeranyl acetate

Inchi: InChI=1S/C12H20O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6H,3,5,7-9H2,1-2,4H3
InchiKey: CVMCLMIPPLWKLI-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=C(CCC=C(C)C)CCOC(C)=O
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-32.80	kJ/mol	Joback Method
hf	-312.74	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	50.91	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1276.00		NIST Webbook
tb	550.85	K	Joback Method
tc	736.37	K	Joback Method
tf	262.40	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.51	J/mol×K	550.85	Joback Method
cpg	440.72	J/mol×K	581.77	Joback Method
cpg	455.22	J/mol×K	612.69	Joback Method
cpg	469.03	J/mol×K	643.61	Joback Method
cpg	482.17	J/mol×K	674.53	Joback Method
cpg	494.67	J/mol×K	705.45	Joback Method
cpg	506.56	J/mol×K	736.37	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=R134020&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