Geranyl isohexanoate

Inchi: InChI=1S/C16H28O2/c1-13(2)7-6-8-15(5)11-12-18-16(17)10-9-14(3)4/h7,11,14H,6,8-10,
InchiKey: DUFDVHTVEPGEQM-PTNGSMBKSA-N
Formula: C16H28O2
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(C)C
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	-9.18	kJ/mol	Joback Method
hf	-408.79	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.659		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	649.41	K	Joback Method
tc	834.76	K	Joback Method
tf	289.16	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.96	J/mol×K	649.41	Joback Method
cpg	651.71	J/mol×K	680.30	Joback Method
cpg	668.60	J/mol×K	711.19	Joback Method
cpg	684.64	J/mol×K	742.09	Joback Method
cpg	699.90	J/mol×K	772.98	Joback Method
cpg	714.39	J/mol×K	803.87	Joback Method
cpg	728.16	J/mol×K	834.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200672&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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