Geranyl isoheptanoate

Inchi: InChI=1S/C17H30O2/c1-14(2)8-6-10-16(5)12-13-19-17(18)11-7-9-15(3)4/h8,12,15H,6-7,
InchiKey: ZKNPBCUOCULKRL-VBKFSLOCSA-N
Formula: C17H30O2
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCCC(C)C
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	-0.76	kJ/mol	Joback Method
hf	-429.43	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	5.049		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	672.29	K	Joback Method
tc	856.36	K	Joback Method
tf	300.43	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.18	J/mol×K	672.29	Joback Method
cpg	707.31	J/mol×K	702.97	Joback Method
cpg	724.55	J/mol×K	733.65	Joback Method
cpg	740.94	J/mol×K	764.33	Joback Method
cpg	756.52	J/mol×K	795.01	Joback Method
cpg	771.33	J/mol×K	825.69	Joback Method
cpg	785.40	J/mol×K	856.36	Joback Method

Sources

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=R200667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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