Geranyl oleate

Inchi: InChI=1S/C28H50O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2
InchiKey: QCKYQBHVRCICQS-VBHPUSIBSA-N
Formula: C28H50O2
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 418.70
CAS: 81601-03-8

Physical Properties

Property code	Value	Unit	Source
gf	174.52	kJ/mol	Joback Method
hf	-533.97	kJ/mol	Joback Method
hfus	69.05	kJ/mol	Joback Method
hvap	87.11	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	9.260		Crippen Method
mcvol	399.920	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	2926.20		NIST Webbook
rinpol	2926.20		NIST Webbook
tb	928.57	K	Joback Method
tc	1137.70	K	Joback Method
tf	434.32	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1334.49	J/mol×K	928.57	Joback Method
cpg	1356.85	J/mol×K	963.43	Joback Method
cpg	1378.09	J/mol×K	998.28	Joback Method
cpg	1398.32	J/mol×K	1033.14	Joback Method
cpg	1417.64	J/mol×K	1067.99	Joback Method
cpg	1436.15	J/mol×K	1102.85	Joback Method
cpg	1453.97	J/mol×K	1137.70	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=C81601038&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