Sebacic acid, geranyl heptyl ester

Inchi: InChI=1S/C27H48O4/c1-5-6-7-12-15-22-30-26(28)19-13-10-8-9-11-14-20-27(29)31-23-2
InchiKey: FFZSNJLZBLBMPJ-NJNXFGOHSA-N
Formula: C27H48O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-148.04	kJ/mol	Joback Method
hf	-875.35	kJ/mol	Joback Method
hfus	69.04	kJ/mol	Joback Method
hvap	94.08	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.857		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	769.89	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	977.82	K	Joback Method
tc	1201.42	K	Joback Method
tf	500.29	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.09	J/mol×K	977.82	Joback Method
cpg	1373.85	J/mol×K	1015.09	Joback Method
cpg	1393.20	J/mol×K	1052.35	Joback Method
cpg	1411.25	J/mol×K	1089.62	Joback Method
cpg	1428.08	J/mol×K	1126.88	Joback Method
cpg	1443.77	J/mol×K	1164.15	Joback Method
cpg	1458.42	J/mol×K	1201.42	Joback Method

Sources

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=U356103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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