Sebacic acid, geranyl isobutyl ester

Inchi: InChI=1S/C24H42O4/c1-20(2)13-12-14-22(5)17-18-27-23(25)15-10-8-6-7-9-11-16-24(26
InchiKey: JMWDXLBOPAWUOD-OQKWZONESA-N
Formula: C24H42O4
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-175.74	kJ/mol	Joback Method
hf	-818.71	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.542		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	913.84	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	908.74	K	Joback Method
tc	1112.69	K	Joback Method
tf	451.48	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.03	J/mol×K	908.74	Joback Method
cpg	1182.01	J/mol×K	942.73	Joback Method
cpg	1199.83	J/mol×K	976.72	Joback Method
cpg	1216.53	J/mol×K	1010.71	Joback Method
cpg	1232.18	J/mol×K	1044.71	Joback Method
cpg	1246.83	J/mol×K	1078.70	Joback Method
cpg	1260.55	J/mol×K	1112.69	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=U356098&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