Sebacic acid, geranyl propyl ester

Inchi: InChI=1S/C23H40O4/c1-5-18-26-22(24)15-10-8-6-7-9-11-16-23(25)27-19-17-21(4)14-12
InchiKey: NHDOBNIBFGIIHE-HEHNFIMWSA-N
Formula: C23H40O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-181.72	kJ/mol	Joback Method
hf	-792.79	kJ/mol	Joback Method
hfus	58.68	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.296		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	964.47	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	886.30	K	Joback Method
tc	1085.70	K	Joback Method
tf	455.21	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.28	J/mol×K	886.30	Joback Method
cpg	1118.82	J/mol×K	919.53	Joback Method
cpg	1136.26	J/mol×K	952.77	Joback Method
cpg	1152.65	J/mol×K	986.00	Joback Method
cpg	1168.05	J/mol×K	1019.23	Joback Method
cpg	1182.50	J/mol×K	1052.47	Joback Method
cpg	1196.06	J/mol×K	1085.70	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=U356097&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