Sebacic acid, geranyl pentyl ester

Inchi: InChI=1S/C25H44O4/c1-5-6-13-20-28-24(26)17-11-9-7-8-10-12-18-25(27)29-21-19-23(4
InchiKey: UVEHGSUFXDGKEJ-FCDQGJHFSA-N
Formula: C25H44O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-164.88	kJ/mol	Joback Method
hf	-834.07	kJ/mol	Joback Method
hfus	63.86	kJ/mol	Joback Method
hvap	89.63	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	2849.00		NIST Webbook
tb	932.06	K	Joback Method
tc	1141.47	K	Joback Method
tf	477.75	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.54	J/mol×K	932.06	Joback Method
cpg	1245.08	J/mol×K	966.96	Joback Method
cpg	1263.38	J/mol×K	1001.86	Joback Method
cpg	1280.53	J/mol×K	1036.76	Joback Method
cpg	1296.58	J/mol×K	1071.67	Joback Method
cpg	1311.60	J/mol×K	1106.57	Joback Method
cpg	1325.65	J/mol×K	1141.47	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=U356100&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