Sebacic acid, geranyl nonyl ester

Inchi: InChI=1S/C29H52O4/c1-5-6-7-8-11-14-17-24-32-28(30)21-15-12-9-10-13-16-22-29(31)3
InchiKey: NOOKRYPJQVSZJL-SLEBQGDGSA-N
Formula: C29H52O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-916.63	kJ/mol	Joback Method
hfus	74.22	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.637		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	693.98	kPa	Joback Method
rinpol	3248.00		NIST Webbook
tb	1023.58	K	Joback Method
tc	1266.21	K	Joback Method
tf	522.83	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.57	J/mol×K	1023.58	Joback Method
cpg	1504.83	J/mol×K	1064.02	Joback Method
cpg	1525.47	J/mol×K	1104.46	Joback Method
cpg	1544.62	J/mol×K	1144.90	Joback Method
cpg	1562.39	J/mol×K	1185.34	Joback Method
cpg	1578.90	J/mol×K	1225.77	Joback Method
cpg	1594.29	J/mol×K	1266.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356105&Units=SI
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

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