Sebacic acid, geranyl undecyl ester

Inchi: InChI=1S/C31H56O4/c1-5-6-7-8-9-10-13-16-19-26-34-30(32)23-17-14-11-12-15-18-24-3
InchiKey: SHJCZEHSBOFEON-XLVZBRSZSA-N
Formula: C31H56O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-114.36	kJ/mol	Joback Method
hf	-957.91	kJ/mol	Joback Method
hfus	79.40	kJ/mol	Joback Method
hvap	102.99	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	9.417		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	628.77	kPa	Joback Method
rinpol	3455.00		NIST Webbook
rinpol	3455.00		NIST Webbook
tb	1069.34	K	Joback Method
tc	1336.66	K	Joback Method
tf	545.37	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1613.68	J/mol×K	1069.34	Joback Method
cpg	1637.79	J/mol×K	1113.89	Joback Method
cpg	1659.99	J/mol×K	1158.45	Joback Method
cpg	1680.48	J/mol×K	1203.00	Joback Method
cpg	1699.41	J/mol×K	1247.55	Joback Method
cpg	1716.98	J/mol×K	1292.11	Joback Method
cpg	1733.34	J/mol×K	1336.66	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=U356107&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