Sebacic acid, geranyl octyl ester

Inchi: InChI=1S/C28H50O4/c1-5-6-7-8-13-16-23-31-27(29)20-14-11-9-10-12-15-21-28(30)32-2
InchiKey: JSJWROOUELPWER-XTCLZLMSSA-N
Formula: C28H50O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-895.99	kJ/mol	Joback Method
hfus	71.63	kJ/mol	Joback Method
hvap	96.31	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.247		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	730.46	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	1000.70	K	Joback Method
tc	1233.16	K	Joback Method
tf	511.56	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.61	J/mol×K	1000.70	Joback Method
cpg	1439.08	J/mol×K	1039.44	Joback Method
cpg	1459.04	J/mol×K	1078.19	Joback Method
cpg	1477.61	J/mol×K	1116.93	Joback Method
cpg	1494.89	J/mol×K	1155.67	Joback Method
cpg	1510.97	J/mol×K	1194.42	Joback Method
cpg	1525.96	J/mol×K	1233.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356104&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