Succinic acid, 2,2-dichloroethyl geranyl ester

Inchi: InChI=1S/C16H24Cl2O4/c1-12(2)5-4-6-13(3)9-10-21-15(19)7-8-16(20)22-11-14(17)18/h5
InchiKey: OLLMSDFYNCTPLD-UKTHLTGXSA-N
Formula: C16H24Cl2O4
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 351.26

Physical Properties

Property code	Value	Unit	Source
gf	-266.96	kJ/mol	Joback Method
hf	-685.07	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.349		Crippen Method
mcvol	267.060	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	800.56	K	Joback Method
tc	1001.01	K	Joback Method
tf	421.16	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.81	J/mol×K	800.56	Joback Method
cpg	756.95	J/mol×K	833.97	Joback Method
cpg	770.22	J/mol×K	867.38	Joback Method
cpg	782.68	J/mol×K	900.79	Joback Method
cpg	794.35	J/mol×K	934.20	Joback Method
cpg	805.28	J/mol×K	967.60	Joback Method
cpg	815.50	J/mol×K	1001.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391211&Units=SI

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