Succinic acid, 1,1,1-trifluoroprop-2-yl pentachlorophenyl ester

Inchi: InChI=1S/C13H8Cl5F3O4/c1-4(13(19,20)21)24-5(22)2-3-6(23)25-12-10(17)8(15)7(14)9(1

InchiKey: FRWALXJVJAHYSR-UHFFFAOYSA-N

Formula: C13H8Cl5F3O4

SMILES: CC(OC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)C(F)(F)F

Mol. weight [g/mol]: 462.46

Physical Properties

Property code	Value	Unit	Source
gf	-988.68	kJ/mol	Joback Method
hf	-1303.13	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.133		Crippen Method
mcvol	251.660	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	882.29	K	Joback Method
tc	1101.69	K	Joback Method
tf	608.40	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.37	J/mol×K	882.29	Joback Method
cpg	622.65	J/mol×K	918.86	Joback Method
cpg	629.11	J/mol×K	955.42	Joback Method
cpg	634.76	J/mol×K	991.99	Joback Method
cpg	639.61	J/mol×K	1028.55	Joback Method
cpg	643.69	J/mol×K	1065.12	Joback Method
cpg	646.99	J/mol×K	1101.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390043&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