Succinic acid, 2,2,3,3-tetrafluoropropyl pentachlorophenyl ester

Inchi: InChI=1S/C13H7Cl5F4O4/c14-6-7(15)9(17)11(10(18)8(6)16)26-5(24)2-1-4(23)25-3-13(21

InchiKey: UGFYADCVBQYQPG-UHFFFAOYSA-N

Formula: C13H7Cl5F4O4

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

Mol. weight [g/mol]: 480.45

Physical Properties

Property code	Value	Unit	Source
gf	-1183.49	kJ/mol	Joback Method
hf	-1499.24	kJ/mol	Joback Method
hfus	49.46	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.083		Crippen Method
mcvol	253.430	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2411.00		NIST Webbook
tb	881.56	K	Joback Method
tc	1095.63	K	Joback Method
tf	608.99	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.78	J/mol×K	881.56	Joback Method
cpg	629.77	J/mol×K	917.24	Joback Method
cpg	635.97	J/mol×K	952.92	Joback Method
cpg	641.39	J/mol×K	988.59	Joback Method
cpg	646.06	J/mol×K	1024.27	Joback Method
cpg	649.98	J/mol×K	1059.95	Joback Method
cpg	653.17	J/mol×K	1095.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390044&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