Succinic acid, 1,1,1-trifluoroprop-2-yl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C13H10Cl3F3O4/c1-6(13(17,18)19)22-10(20)2-3-11(21)23-12-8(15)4-7(14)5-9

InchiKey: YMGFMZRWMWHJLR-UHFFFAOYSA-N

Formula: C13H10Cl3F3O4

SMILES: CC(OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)C(F)(F)F

Mol. weight [g/mol]: 393.57

Physical Properties

Property code	Value	Unit	Source
gf	-945.56	kJ/mol	Joback Method
hf	-1248.71	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.826		Crippen Method
mcvol	227.180	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	797.47	K	Joback Method
tc	1007.71	K	Joback Method
tf	523.52	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.70	J/mol×K	797.47	Joback Method
cpg	591.17	J/mol×K	832.51	Joback Method
cpg	599.82	J/mol×K	867.55	Joback Method
cpg	607.66	J/mol×K	902.59	Joback Method
cpg	614.72	J/mol×K	937.63	Joback Method
cpg	621.03	J/mol×K	972.67	Joback Method
cpg	626.59	J/mol×K	1007.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390267&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