Succinic acid, 2-chloro-6-fluorophenyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H9Cl4FO4/c13-7-2-1-3-8(17)11(7)21-10(19)5-4-9(18)20-6-12(14,15)16/h1-

InchiKey: AXTRJRLXJSAMRG-UHFFFAOYSA-N

Formula: C12H9Cl4FO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 378.01

Physical Properties

Property code	Value	Unit	Source
gf	-564.22	kJ/mol	Joback Method
hf	-834.84	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.078		Crippen Method
mcvol	221.790	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2209.00		NIST Webbook
tb	808.94	K	Joback Method
tc	1035.61	K	Joback Method
tf	543.47	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.72	J/mol×K	808.94	Joback Method
cpg	543.46	J/mol×K	846.72	Joback Method
cpg	551.35	J/mol×K	884.50	Joback Method
cpg	558.41	J/mol×K	922.28	Joback Method
cpg	564.68	J/mol×K	960.05	Joback Method
cpg	570.18	J/mol×K	997.83	Joback Method
cpg	574.95	J/mol×K	1035.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390238&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