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

Inchi: InChI=1S/C12H10Cl3FO4/c13-7-2-1-3-8(16)12(7)20-11(18)5-4-10(17)19-6-9(14)15/h1-3,

InchiKey: NLOAJHQHHMQUGI-UHFFFAOYSA-N

Formula: C12H10Cl3FO4

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

Mol. weight [g/mol]: 343.56

Physical Properties

Property code	Value	Unit	Source
gf	-557.57	kJ/mol	Joback Method
hf	-815.63	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.512		Crippen Method
mcvol	209.550	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	774.30	K	Joback Method
tc	991.65	K	Joback Method
tf	496.13	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.24	J/mol×K	774.30	Joback Method
cpg	523.13	J/mol×K	810.52	Joback Method
cpg	532.18	J/mol×K	846.75	Joback Method
cpg	540.39	J/mol×K	882.97	Joback Method
cpg	547.78	J/mol×K	919.20	Joback Method
cpg	554.33	J/mol×K	955.42	Joback Method
cpg	560.07	J/mol×K	991.65	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=U390521&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