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

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

InchiKey: QVWVXTQTBISWHF-UHFFFAOYSA-N

Formula: C12H10Cl3FO4

SMILES: O=C(CCC(=O)Oc1ccccc1F)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 343.56

Physical Properties

Property code	Value	Unit	Source
gf	-542.66	kJ/mol	Joback Method
hf	-807.63	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	74.60	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.425		Crippen Method
mcvol	209.550	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	766.53	K	Joback Method
tc	989.61	K	Joback Method
tf	501.03	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.80	J/mol×K	766.53	Joback Method
cpg	526.73	J/mol×K	803.71	Joback Method
cpg	535.77	J/mol×K	840.89	Joback Method
cpg	543.96	J/mol×K	878.07	Joback Method
cpg	551.33	J/mol×K	915.25	Joback Method
cpg	557.91	J/mol×K	952.43	Joback Method
cpg	563.74	J/mol×K	989.61	Joback Method

Sources

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=U390235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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