Succinic acid, 2,2-dichloroethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C13H13Cl2FO5/c1-19-10-6-8(16)2-3-9(10)21-13(18)5-4-12(17)20-7-11(14)15/h

InchiKey: GJNUDBKKMAASDY-UHFFFAOYSA-N

Formula: C13H13Cl2FO5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 339.14

Physical Properties

Property code	Value	Unit	Source
gf	-642.22	kJ/mol	Joback Method
hf	-952.75	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.867		Crippen Method
mcvol	217.270	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	782.17	K	Joback Method
tc	992.42	K	Joback Method
tf	499.71	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.00	J/mol×K	782.17	Joback Method
cpg	580.11	J/mol×K	817.21	Joback Method
cpg	590.30	J/mol×K	852.25	Joback Method
cpg	599.58	J/mol×K	887.30	Joback Method
cpg	607.94	J/mol×K	922.34	Joback Method
cpg	615.35	J/mol×K	957.38	Joback Method
cpg	621.82	J/mol×K	992.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390901&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