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

Inchi: InChI=1S/C12H11Cl2FO4/c13-10(14)7-18-11(16)5-6-12(17)19-9-4-2-1-3-8(9)15/h1-4,10H

InchiKey: MEFDKKDUDUPKPH-UHFFFAOYSA-N

Formula: C12H11Cl2FO4

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

Mol. weight [g/mol]: 309.12

Physical Properties

Property code	Value	Unit	Source
gf	-536.01	kJ/mol	Joback Method
hf	-788.42	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.858		Crippen Method
mcvol	197.310	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	731.89	K	Joback Method
tc	945.29	K	Joback Method
tf	453.69	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.23	J/mol×K	731.89	Joback Method
cpg	504.25	J/mol×K	767.46	Joback Method
cpg	514.44	J/mol×K	803.02	Joback Method
cpg	523.79	J/mol×K	838.59	Joback Method
cpg	532.33	J/mol×K	874.16	Joback Method
cpg	540.05	J/mol×K	909.73	Joback Method
cpg	546.96	J/mol×K	945.29	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=U390307&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