Succinic acid, 2-chloro-6-fluorophenyl 2-chloro-4-methylphenyl ester

Inchi: InChI=1S/C17H13Cl2FO4/c1-10-5-6-14(12(19)9-10)23-15(21)7-8-16(22)24-17-11(18)3-2

InchiKey: XJFSJUHMMYWXOT-UHFFFAOYSA-N

Formula: C17H13Cl2FO4

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2c(F)cccc2Cl)c(Cl)c1

Mol. weight [g/mol]: 371.19

Physical Properties

Property code	Value	Unit	Source
gf	-407.95	kJ/mol	Joback Method
hf	-684.22	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.732		Crippen Method
mcvol	244.000	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	888.35	K	Joback Method
tc	1120.07	K	Joback Method
tf	589.02	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.26	J/mol×K	888.35	Joback Method
cpg	669.53	J/mol×K	926.97	Joback Method
cpg	678.65	J/mol×K	965.59	Joback Method
cpg	686.63	J/mol×K	1004.21	Joback Method
cpg	693.48	J/mol×K	1042.83	Joback Method
cpg	699.23	J/mol×K	1081.45	Joback Method
cpg	703.87	J/mol×K	1120.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390220&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

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