Succinic acid, 2,3-dichlorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C16H11Cl2FO4/c17-12-5-2-6-13(16(12)18)23-15(21)8-7-14(20)22-11-4-1-3-10

InchiKey: ZFYFGMWGOUJBMX-UHFFFAOYSA-N

Formula: C16H11Cl2FO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1cccc(F)c1

Mol. weight [g/mol]: 357.16

Physical Properties

Property code	Value	Unit	Source
gf	-406.74	kJ/mol	Joback Method
hf	-652.11	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	84.01	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.424		Crippen Method
mcvol	229.910	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	860.49	K	Joback Method
tc	1094.08	K	Joback Method
tf	565.23	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.09	J/mol×K	860.49	Joback Method
cpg	616.21	J/mol×K	899.42	Joback Method
cpg	625.23	J/mol×K	938.35	Joback Method
cpg	633.14	J/mol×K	977.29	Joback Method
cpg	639.98	J/mol×K	1016.22	Joback Method
cpg	645.76	J/mol×K	1055.15	Joback Method
cpg	650.51	J/mol×K	1094.08	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=U390337&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