Succinic acid, 3,5-difluorophenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C16H10Cl2F2O4/c17-12-2-1-3-13(16(12)18)24-15(22)5-4-14(21)23-11-7-9(19)6-10(20)8-11/h1-3,6-8H,4-5H2

InchiKey: NYLQGKLONLUHMQ-UHFFFAOYSA-N

Formula: C16H10Cl2F2O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 375.15

Physical Properties

Property code	Value	Unit	Source
gf	-611.18	kJ/mol	Joback Method
hf	-859.69	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.563		Crippen Method
mcvol	231.680	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2502.00		NIST Webbook
tb	864.74	K	Joback Method
tc	1091.58	K	Joback Method
tf	578.34	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.78	J/mol×K	864.74	Joback Method
cpg	621.38	J/mol×K	902.55	Joback Method
cpg	629.92	J/mol×K	940.35	Joback Method
cpg	637.43	J/mol×K	978.16	Joback Method
cpg	643.90	J/mol×K	1015.97	Joback Method
cpg	649.35	J/mol×K	1053.78	Joback Method
cpg	653.79	J/mol×K	1091.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358039&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

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