Succinic acid, 2,3-dichlorophenyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C17H10Cl2F4O4/c18-10-4-2-5-11(15(10)19)26-13(24)7-8-14(25)27-12-6-1-3-9

InchiKey: BNERIOBYOVUPBC-UHFFFAOYSA-N

Formula: C17H10Cl2F4O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 425.16

Physical Properties

Property code	Value	Unit	Source
gf	-989.54	kJ/mol	Joback Method
hf	-1281.30	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	83.15	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.442		Crippen Method
mcvol	249.310	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	882.93	K	Joback Method
tc	1103.08	K	Joback Method
tf	593.21	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.60	J/mol×K	882.93	Joback Method
cpg	691.77	J/mol×K	919.62	Joback Method
cpg	699.96	J/mol×K	956.31	Joback Method
cpg	707.21	J/mol×K	993.01	Joback Method
cpg	713.56	J/mol×K	1029.70	Joback Method
cpg	719.04	J/mol×K	1066.39	Joback Method
cpg	723.70	J/mol×K	1103.08	Joback Method

Sources

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=U390791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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