Succinic acid, 2,3-dichlorophenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H9Cl2F3O4/c17-8-2-1-3-10(14(8)18)24-12(22)6-7-13(23)25-11-5-4-9(19)15

InchiKey: AILXGRMDBJMMHP-UHFFFAOYSA-N

Formula: C16H9Cl2F3O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 393.14

Physical Properties

Property code	Value	Unit	Source
gf	-815.62	kJ/mol	Joback Method
hf	-1067.27	kJ/mol	Joback Method
hfus	46.54	kJ/mol	Joback Method
hvap	83.70	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.702		Crippen Method
mcvol	233.450	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	868.99	K	Joback Method
tc	1089.93	K	Joback Method
tf	591.45	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.43	J/mol×K	868.99	Joback Method
cpg	626.55	J/mol×K	905.81	Joback Method
cpg	634.66	J/mol×K	942.64	Joback Method
cpg	641.78	J/mol×K	979.46	Joback Method
cpg	647.91	J/mol×K	1016.28	Joback Method
cpg	653.04	J/mol×K	1053.11	Joback Method
cpg	657.19	J/mol×K	1089.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390769&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