Succinic acid, 2-fluorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H10Cl3FO4/c17-9-7-11(19)14(8-10(9)18)24-16(22)6-5-15(21)23-13-4-2-1-3

InchiKey: UMESFYUVGODDJV-UHFFFAOYSA-N

Formula: C16H10Cl3FO4

SMILES: O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)Oc1ccccc1F

Mol. weight [g/mol]: 391.61

Physical Properties

Property code	Value	Unit	Source
gf	-428.30	kJ/mol	Joback Method
hf	-679.32	kJ/mol	Joback Method
hfus	44.97	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.077		Crippen Method
mcvol	242.150	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	2621.00		NIST Webbook
rinpol	2621.00		NIST Webbook
tb	902.90	K	Joback Method
tc	1140.03	K	Joback Method
tf	607.67	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.99	J/mol×K	902.90	Joback Method
cpg	631.74	J/mol×K	942.42	Joback Method
cpg	639.37	J/mol×K	981.94	Joback Method
cpg	645.90	J/mol×K	1021.46	Joback Method
cpg	651.33	J/mol×K	1060.98	Joback Method
cpg	655.68	J/mol×K	1100.50	Joback Method
cpg	658.96	J/mol×K	1140.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389967&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