Succinic acid, 2-chloro-6-fluorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H9Cl4FO4/c17-8-2-1-3-12(21)16(8)25-15(23)5-4-14(22)24-13-7-10(19)9(18

InchiKey: JVKGVFFDZSVRHU-UHFFFAOYSA-N

Formula: C16H9Cl4FO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 426.05

Physical Properties

Property code	Value	Unit	Source
gf	-449.86	kJ/mol	Joback Method
hf	-706.53	kJ/mol	Joback Method
hfus	48.77	kJ/mol	Joback Method
hvap	94.11	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.730		Crippen Method
mcvol	254.390	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	945.31	K	Joback Method
tc	1186.15	K	Joback Method
tf	650.11	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.96	J/mol×K	945.31	Joback Method
cpg	645.33	J/mol×K	985.45	Joback Method
cpg	651.56	J/mol×K	1025.59	Joback Method
cpg	656.66	J/mol×K	1065.73	Joback Method
cpg	660.63	J/mol×K	1105.87	Joback Method
cpg	663.49	J/mol×K	1146.01	Joback Method
cpg	665.23	J/mol×K	1186.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389970&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