Succinic acid, 2-chloro-6-fluorophenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H9ClF4O4/c17-8-2-1-3-10(19)16(8)25-13(23)7-6-12(22)24-11-5-4-9(18)14(

InchiKey: YOGWCONZQFPBAB-UHFFFAOYSA-N

Formula: C16H9ClF4O4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 376.69

Physical Properties

Property code	Value	Unit	Source
gf	-998.50	kJ/mol	Joback Method
hf	-1247.64	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.188		Crippen Method
mcvol	222.980	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2243.00		NIST Webbook
tb	830.83	K	Joback Method
tc	1041.85	K	Joback Method
tf	562.12	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.08	J/mol×K	830.83	Joback Method
cpg	614.96	J/mol×K	866.00	Joback Method
cpg	623.92	J/mol×K	901.17	Joback Method
cpg	631.94	J/mol×K	936.34	Joback Method
cpg	639.05	J/mol×K	971.51	Joback Method
cpg	645.22	J/mol×K	1006.68	Joback Method
cpg	650.48	J/mol×K	1041.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390765&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