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

Inchi: InChI=1S/C16H10ClF3O4/c17-9-2-1-3-10(8-9)23-13(21)6-7-14(22)24-12-5-4-11(18)15(19

InchiKey: PJZIMHCUERCVBS-UHFFFAOYSA-N

Formula: C16H10ClF3O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 358.70

Physical Properties

Property code	Value	Unit	Source
gf	-794.06	kJ/mol	Joback Method
hf	-1040.06	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.048		Crippen Method
mcvol	221.210	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	826.58	K	Joback Method
tc	1043.17	K	Joback Method
tf	549.01	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.16	J/mol×K	826.58	Joback Method
cpg	609.53	J/mol×K	862.68	Joback Method
cpg	618.92	J/mol×K	898.78	Joback Method
cpg	627.34	J/mol×K	934.87	Joback Method
cpg	634.79	J/mol×K	970.97	Joback Method
cpg	641.29	J/mol×K	1007.07	Joback Method
cpg	646.83	J/mol×K	1043.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390766&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