Succinic acid, 4-chloro-3-methylphenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H12ClF3O4/c1-9-8-10(2-3-11(9)18)24-14(22)6-7-15(23)25-13-5-4-12(19)16(20)17(13)21

InchiKey: HZPAQPFRJBXXLX-UHFFFAOYSA-N

Formula: C17H12ClF3O4

SMILES: Cc1cc(OC(=O)CCC(=O)Oc2ccc(F)c(F)c2F)ccc1Cl

Mol. weight [g/mol]: 372.72

Physical Properties

Property code	Value	Unit	Source
gf	-795.27	kJ/mol	Joback Method
hf	-1072.17	kJ/mol	Joback Method
hfus	44.93	kJ/mol	Joback Method
hvap	81.54	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.357		Crippen Method
mcvol	235.300	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	854.44	K	Joback Method
tc	1070.35	K	Joback Method
tf	572.80	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.11	J/mol×K	854.44	Joback Method
cpg	662.70	J/mol×K	890.42	Joback Method
cpg	672.26	J/mol×K	926.41	Joback Method
cpg	680.80	J/mol×K	962.39	Joback Method
cpg	688.33	J/mol×K	998.38	Joback Method
cpg	694.84	J/mol×K	1034.36	Joback Method
cpg	700.34	J/mol×K	1070.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390768&Units=SI

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