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

Inchi: InChI=1S/C17H14ClFO4/c1-11-10-12(6-7-13(11)18)22-16(20)8-9-17(21)23-15-5-3-2-4-14

InchiKey: XYCMUMPIRJGUOX-UHFFFAOYSA-N

Formula: C17H14ClFO4

SMILES: Cc1cc(OC(=O)CCC(=O)Oc2ccccc2F)ccc1Cl

Mol. weight [g/mol]: 336.74

Physical Properties

Property code	Value	Unit	Source
gf	-386.39	kJ/mol	Joback Method
hf	-657.01	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.079		Crippen Method
mcvol	231.760	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	845.94	K	Joback Method
tc	1073.89	K	Joback Method
tf	546.58	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.27	J/mol×K	845.94	Joback Method
cpg	651.94	J/mol×K	883.93	Joback Method
cpg	662.46	J/mol×K	921.92	Joback Method
cpg	671.86	J/mol×K	959.91	Joback Method
cpg	680.16	J/mol×K	997.91	Joback Method
cpg	687.36	J/mol×K	1035.90	Joback Method
cpg	693.50	J/mol×K	1073.89	Joback Method

Sources

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=U390313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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