Succinic acid, 2-fluorophenyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H14ClFO5/c1-22-15-10-11(18)6-7-14(15)24-17(21)9-8-16(20)23-13-5-3-2-4

InchiKey: DGIOJXJGVSTXMC-UHFFFAOYSA-N

Formula: C17H14ClFO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 352.74

Physical Properties

Property code	Value	Unit	Source
gf	-491.39	kJ/mol	Joback Method
hf	-789.23	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.779		Crippen Method
mcvol	237.630	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	868.36	K	Joback Method
tc	1094.78	K	Joback Method
tf	568.81	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.73	J/mol×K	868.36	Joback Method
cpg	676.82	J/mol×K	906.10	Joback Method
cpg	686.68	J/mol×K	943.83	Joback Method
cpg	695.31	J/mol×K	981.57	Joback Method
cpg	702.72	J/mol×K	1019.31	Joback Method
cpg	708.90	J/mol×K	1057.04	Joback Method
cpg	713.86	J/mol×K	1094.78	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=U390938&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