Succinic acid, 4-chloro-3-methylphenyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H16ClFO5/c1-11-9-13(4-5-14(11)19)24-17(21)7-8-18(22)25-15-6-3-12(20)

InchiKey: OTCBJTWCBXKYGQ-UHFFFAOYSA-N

Formula: C18H16ClFO5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 366.77

Physical Properties

Property code	Value	Unit	Source
gf	-492.60	kJ/mol	Joback Method
hf	-821.34	kJ/mol	Joback Method
hfus	42.94	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.087		Crippen Method
mcvol	251.720	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2577.00		NIST Webbook
rinpol	2577.00		NIST Webbook
tb	896.22	K	Joback Method
tc	1121.70	K	Joback Method
tf	592.60	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.05	J/mol×K	896.22	Joback Method
cpg	731.17	J/mol×K	933.80	Joback Method
cpg	741.00	J/mol×K	971.38	Joback Method
cpg	749.55	J/mol×K	1008.96	Joback Method
cpg	756.81	J/mol×K	1046.54	Joback Method
cpg	762.78	J/mol×K	1084.12	Joback Method
cpg	767.44	J/mol×K	1121.70	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=U390907&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