Succinic acid, 2-chloro-6-fluorophenyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H13ClF2O5/c1-23-14-9-10(19)5-6-13(14)24-15(21)7-8-16(22)25-17-11(18)3-2-4-12(17)20/h2-6,9H,7-8H2,1H3

InchiKey: UCTVNSHFNIVOCM-UHFFFAOYSA-N

Formula: C17H13ClF2O5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 370.73

Physical Properties

Property code	Value	Unit	Source
gf	-695.83	kJ/mol	Joback Method
hf	-996.81	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	84.11	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.918		Crippen Method
mcvol	239.400	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	872.61	K	Joback Method
tc	1093.26	K	Joback Method
tf	581.92	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.55	J/mol×K	872.61	Joback Method
cpg	682.10	J/mol×K	909.38	Joback Method
cpg	691.49	J/mol×K	946.16	Joback Method
cpg	699.70	J/mol×K	982.93	Joback Method
cpg	706.73	J/mol×K	1019.71	Joback Method
cpg	712.58	J/mol×K	1056.48	Joback Method
cpg	717.23	J/mol×K	1093.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390906&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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