Succinic acid, 2-chloro-6-fluorophenyl 4-methoxybenzyl ester

Inchi: InChI=1S/C18H16ClFO5/c1-23-13-7-5-12(6-8-13)11-24-16(21)9-10-17(22)25-18-14(19)3

InchiKey: WPWGKTMZNLMUEE-UHFFFAOYSA-N

Formula: C18H16ClFO5

SMILES: COc1ccc(COC(=O)CCC(=O)Oc2c(F)cccc2Cl)cc1

Mol. weight [g/mol]: 366.77

Physical Properties

Property code	Value	Unit	Source
gf	-482.97	kJ/mol	Joback Method
hf	-809.87	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.917		Crippen Method
mcvol	251.720	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		NIST Webbook
tb	891.24	K	Joback Method
tc	1115.95	K	Joback Method
tf	580.08	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.57	J/mol×K	891.24	Joback Method
cpg	732.80	J/mol×K	928.69	Joback Method
cpg	742.76	J/mol×K	966.14	Joback Method
cpg	751.45	J/mol×K	1003.60	Joback Method
cpg	758.89	J/mol×K	1041.05	Joback Method
cpg	765.07	J/mol×K	1078.50	Joback Method
cpg	770.01	J/mol×K	1115.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389692&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