Succinic acid, 2-chloro-6-fluorophenyl 1-phenylpropyl ester

Inchi: InChI=1S/C19H18ClFO4/c1-2-16(13-7-4-3-5-8-13)24-17(22)11-12-18(23)25-19-14(20)9-6

InchiKey: ZPIBLXWRPXVQSH-UHFFFAOYSA-N

Formula: C19H18ClFO4

SMILES: CCC(OC(=O)CCC(=O)Oc1c(F)cccc1Cl)c1ccccc1

Mol. weight [g/mol]: 364.80

Physical Properties

Property code	Value	Unit	Source
gf	-362.36	kJ/mol	Joback Method
hf	-692.10	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.859		Crippen Method
mcvol	259.940	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	886.28	K	Joback Method
tc	1112.24	K	Joback Method
tf	541.60	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.10	J/mol×K	886.28	Joback Method
cpg	766.34	J/mol×K	923.94	Joback Method
cpg	777.35	J/mol×K	961.60	Joback Method
cpg	787.16	J/mol×K	999.26	Joback Method
cpg	795.81	J/mol×K	1036.92	Joback Method
cpg	803.31	J/mol×K	1074.58	Joback Method
cpg	809.72	J/mol×K	1112.24	Joback Method

Sources

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=U389932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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