Succinic acid, 2-chloro-6-fluorophenyl 3-phenylpropyl ester

Inchi: InChI=1S/C19H18ClFO4/c20-15-9-4-10-16(21)19(15)25-18(23)12-11-17(22)24-13-5-8-14

InchiKey: GRLHNEGHFRIDEE-UHFFFAOYSA-N

Formula: C19H18ClFO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCCCc1ccccc1

Mol. weight [g/mol]: 364.80

Physical Properties

Property code	Value	Unit	Source
gf	-359.92	kJ/mol	Joback Method
hf	-686.82	kJ/mol	Joback Method
hfus	45.12	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.341		Crippen Method
mcvol	259.940	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	886.72	K	Joback Method
tc	1110.00	K	Joback Method
tf	556.60	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.55	J/mol×K	886.72	Joback Method
cpg	765.68	J/mol×K	923.93	Joback Method
cpg	776.62	J/mol×K	961.15	Joback Method
cpg	786.40	J/mol×K	998.36	Joback Method
cpg	795.05	J/mol×K	1035.57	Joback Method
cpg	802.61	J/mol×K	1072.78	Joback Method
cpg	809.11	J/mol×K	1110.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389731&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

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