Succinic acid, 2-chloro-6-fluorophenyl phenethyl ester

Inchi: InChI=1S/C18H16ClFO4/c19-14-7-4-8-15(20)18(14)24-17(22)10-9-16(21)23-12-11-13-5-

InchiKey: NNKHYVOTLUDOHV-UHFFFAOYSA-N

Formula: C18H16ClFO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCCc1ccccc1

Mol. weight [g/mol]: 350.77

Physical Properties

Property code	Value	Unit	Source
gf	-368.34	kJ/mol	Joback Method
hf	-666.18	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.951		Crippen Method
mcvol	245.850	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	863.84	K	Joback Method
tc	1088.74	K	Joback Method
tf	545.33	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.25	J/mol×K	863.84	Joback Method
cpg	709.22	J/mol×K	901.32	Joback Method
cpg	720.01	J/mol×K	938.81	Joback Method
cpg	729.68	J/mol×K	976.29	Joback Method
cpg	738.23	J/mol×K	1013.78	Joback Method
cpg	745.71	J/mol×K	1051.26	Joback Method
cpg	752.13	J/mol×K	1088.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389750&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