Succinic acid, 2-chloro-6-fluorophenyl 8-chlorooctyl ester

Inchi: InChI=1S/C18H23Cl2FO4/c19-12-5-3-1-2-4-6-13-24-16(22)10-11-17(23)25-18-14(20)8-7

InchiKey: UTLHIVBQUMYXJV-UHFFFAOYSA-N

Formula: C18H23Cl2FO4

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

Mol. weight [g/mol]: 393.28

Physical Properties

Property code	Value	Unit	Source
gf	-492.68	kJ/mol	Joback Method
hf	-918.45	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.287		Crippen Method
mcvol	281.850	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	874.59	K	Joback Method
tc	1080.14	K	Joback Method
tf	548.83	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.77	J/mol×K	874.59	Joback Method
cpg	832.69	J/mol×K	908.85	Joback Method
cpg	844.57	J/mol×K	943.11	Joback Method
cpg	855.41	J/mol×K	977.37	Joback Method
cpg	865.23	J/mol×K	1011.62	Joback Method
cpg	874.06	J/mol×K	1045.88	Joback Method
cpg	881.92	J/mol×K	1080.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390493&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