Succinic acid, 2-chloro-6-fluorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C20H27Cl2FO4/c21-14-7-5-3-1-2-4-6-8-15-26-18(24)12-13-19(25)27-20-16(22

InchiKey: QIXDNHIDGGLCMJ-UHFFFAOYSA-N

Formula: C20H27Cl2FO4

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

Mol. weight [g/mol]: 421.33

Physical Properties

Property code	Value	Unit	Source
gf	-475.84	kJ/mol	Joback Method
hf	-959.73	kJ/mol	Joback Method
hfus	57.87	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.067		Crippen Method
mcvol	310.030	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	920.35	K	Joback Method
tc	1129.76	K	Joback Method
tf	571.37	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.24	J/mol×K	920.35	Joback Method
cpg	949.67	J/mol×K	955.25	Joback Method
cpg	961.94	J/mol×K	990.15	Joback Method
cpg	973.07	J/mol×K	1025.05	Joback Method
cpg	983.09	J/mol×K	1059.95	Joback Method
cpg	992.02	J/mol×K	1094.86	Joback Method
cpg	999.89	J/mol×K	1129.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390414&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