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

Inchi: InChI=1S/C18H24ClFO4/c1-3-4-5-6-8-13(2)23-16(21)11-12-17(22)24-18-14(19)9-7-10-15

InchiKey: DRROCZVIFHOFSE-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: CCCCCCC(C)OC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-483.19	kJ/mol	Joback Method
hf	-907.99	kJ/mol	Joback Method
hfus	44.97	kJ/mol	Joback Method
hvap	80.75	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.067		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	836.72	K	Joback Method
tc	1038.92	K	Joback Method
tf	503.91	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.44	J/mol×K	836.72	Joback Method
cpg	809.57	J/mol×K	870.42	Joback Method
cpg	822.66	J/mol×K	904.12	Joback Method
cpg	834.71	J/mol×K	937.82	Joback Method
cpg	845.74	J/mol×K	971.52	Joback Method
cpg	855.76	J/mol×K	1005.22	Joback Method
cpg	864.79	J/mol×K	1038.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370978&Units=SI

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