Succinic acid, 2-chloro-6-fluorophenyl oct-1-en-3-yl ester

Inchi: InChI=1S/C18H22ClFO4/c1-3-5-6-8-13(4-2)23-16(21)11-12-17(22)24-18-14(19)9-7-10-15

InchiKey: MHARKZZOYGCYRU-UHFFFAOYSA-N

Formula: C18H22ClFO4

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

Mol. weight [g/mol]: 356.82

Physical Properties

Property code	Value	Unit	Source
gf	-395.35	kJ/mol	Joback Method
hf	-782.56	kJ/mol	Joback Method
hfus	43.69	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.843		Crippen Method
mcvol	265.310	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	833.40	K	Joback Method
tc	1037.32	K	Joback Method
tf	502.15	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.48	J/mol×K	833.40	Joback Method
cpg	782.11	J/mol×K	867.39	Joback Method
cpg	794.73	J/mol×K	901.37	Joback Method
cpg	806.35	J/mol×K	935.36	Joback Method
cpg	816.99	J/mol×K	969.34	Joback Method
cpg	826.67	J/mol×K	1003.33	Joback Method
cpg	835.41	J/mol×K	1037.32	Joback Method

Sources

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=U391322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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