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

Inchi: InChI=1S/C19H24ClFO4/c1-2-3-4-5-6-7-8-14-24-17(22)12-13-18(23)25-19-15(20)10-9-11

InchiKey: XRYFGVNZZBBHCE-VOTSOKGWSA-N

Formula: C19H24ClFO4

SMILES: CCCCCC=CCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 370.84

Physical Properties

Property code	Value	Unit	Source
gf	-392.11	kJ/mol	Joback Method
hf	-806.13	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.234		Crippen Method
mcvol	279.400	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	864.20	K	Joback Method
tc	1069.27	K	Joback Method
tf	525.10	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.68	J/mol×K	864.20	Joback Method
cpg	839.50	J/mol×K	898.38	Joback Method
cpg	852.31	J/mol×K	932.56	Joback Method
cpg	864.14	J/mol×K	966.74	Joback Method
cpg	875.03	J/mol×K	1000.92	Joback Method
cpg	885.00	J/mol×K	1035.09	Joback Method
cpg	894.07	J/mol×K	1069.27	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=U391099&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