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

Inchi: InChI=1S/C14H14ClFO4/c1-2-3-9-19-12(17)7-8-13(18)20-14-10(15)5-4-6-11(14)16/h2,4-

InchiKey: RIMCCNJHGYRISV-UHFFFAOYSA-N

Formula: C14H14ClFO4

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

Mol. weight [g/mol]: 300.71

Physical Properties

Property code	Value	Unit	Source
gf	-426.59	kJ/mol	Joback Method
hf	-694.72	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	71.57	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.284		Crippen Method
mcvol	208.950	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	742.32	K	Joback Method
tc	948.11	K	Joback Method
tf	472.07	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.99	J/mol×K	742.32	Joback Method
cpg	560.08	J/mol×K	776.62	Joback Method
cpg	571.33	J/mol×K	810.92	Joback Method
cpg	581.76	J/mol×K	845.21	Joback Method
cpg	591.38	J/mol×K	879.51	Joback Method
cpg	600.20	J/mol×K	913.81	Joback Method
cpg	608.22	J/mol×K	948.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391196&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