Succinic acid, 2-chloro-6-fluorophenyl but-2-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/h2-6H

InchiKey: SGTSLGVUXCFDJU-NSCUHMNNSA-N

Formula: C14H14ClFO4

SMILES: CC=CCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 300.71

Physical Properties

Property code	Value	Unit	Source
gf	-434.21	kJ/mol	Joback Method
hf	-702.93	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.284		Crippen Method
mcvol	208.950	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	749.80	K	Joback Method
tc	959.11	K	Joback Method
tf	468.75	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.92	J/mol×K	749.80	Joback Method
cpg	560.01	J/mol×K	784.69	Joback Method
cpg	571.26	J/mol×K	819.57	Joback Method
cpg	581.69	J/mol×K	854.46	Joback Method
cpg	591.33	J/mol×K	889.34	Joback Method
cpg	600.18	J/mol×K	924.23	Joback Method
cpg	608.27	J/mol×K	959.11	Joback Method

Sources

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=U391225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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