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

Inchi: InChI=1S/C15H16ClFO4/c1-10(2)8-9-20-13(18)6-7-14(19)21-15-11(16)4-3-5-12(15)17/h3

InchiKey: UPGMUEWCXNHIEC-UHFFFAOYSA-N

Formula: C15H16ClFO4

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

Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
gf	-434.34	kJ/mol	Joback Method
hf	-733.36	kJ/mol	Joback Method
hfus	39.61	kJ/mol	Joback Method
hvap	74.50	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.674		Crippen Method
mcvol	223.040	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	772.56	K	Joback Method
tc	982.37	K	Joback Method
tf	466.06	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.11	J/mol×K	772.56	Joback Method
cpg	613.76	J/mol×K	807.53	Joback Method
cpg	625.52	J/mol×K	842.50	Joback Method
cpg	636.42	J/mol×K	877.46	Joback Method
cpg	646.48	J/mol×K	912.43	Joback Method
cpg	655.72	J/mol×K	947.40	Joback Method
cpg	664.16	J/mol×K	982.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391037&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