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

Inchi: InChI=1S/C15H18ClFO4/c1-9(2)10(3)20-13(18)7-8-14(19)21-15-11(16)5-4-6-12(15)17/h4

InchiKey: QPNSDBJJIMXYMO-UHFFFAOYSA-N

Formula: C15H18ClFO4

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

Mol. weight [g/mol]: 316.75

Physical Properties

Property code	Value	Unit	Source
gf	-510.89	kJ/mol	Joback Method
hf	-851.35	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	73.69	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.752		Crippen Method
mcvol	227.340	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1981.00		NIST Webbook
rinpol	1981.00		NIST Webbook
tb	767.64	K	Joback Method
tc	974.66	K	Joback Method
tf	455.10	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.82	J/mol×K	767.64	Joback Method
cpg	641.27	J/mol×K	802.14	Joback Method
cpg	653.75	J/mol×K	836.65	Joback Method
cpg	665.29	J/mol×K	871.15	Joback Method
cpg	675.87	J/mol×K	905.65	Joback Method
cpg	685.52	J/mol×K	940.15	Joback Method
cpg	694.23	J/mol×K	974.66	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=U390586&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