Succinic acid, 2-chloro-6-fluorophenyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H11ClF4O4/c1-7(13(16,17)18)21-10(19)5-6-11(20)22-12-8(14)3-2-4-9(12)1

InchiKey: TYKLXAZAHIYTFJ-UHFFFAOYSA-N

Formula: C13H11ClF4O4

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

Mol. weight [g/mol]: 342.67

Physical Properties

Property code	Value	Unit	Source
gf	-1106.88	kJ/mol	Joback Method
hf	-1401.87	kJ/mol	Joback Method
hfus	33.84	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.659		Crippen Method
mcvol	204.470	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	716.90	K	Joback Method
tc	912.08	K	Joback Method
tf	451.75	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.76	J/mol×K	716.90	Joback Method
cpg	557.91	J/mol×K	749.43	Joback Method
cpg	568.27	J/mol×K	781.96	Joback Method
cpg	577.88	J/mol×K	814.49	Joback Method
cpg	586.74	J/mol×K	847.02	Joback Method
cpg	594.87	J/mol×K	879.55	Joback Method
cpg	602.30	J/mol×K	912.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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