Succinic acid, 2-chloro-6-fluorophenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H10ClF5O4/c14-7-2-1-3-8(15)11(7)23-10(21)5-4-9(20)22-6-13(18,19)12(16

InchiKey: JIESBOKAEFBTMQ-UHFFFAOYSA-N

Formula: C13H10ClF5O4

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

Mol. weight [g/mol]: 360.66

Physical Properties

Property code	Value	Unit	Source
gf	-1301.69	kJ/mol	Joback Method
hf	-1597.98	kJ/mol	Joback Method
hfus	36.92	kJ/mol	Joback Method
hvap	65.06	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.608		Crippen Method
mcvol	206.240	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	716.17	K	Joback Method
tc	905.02	K	Joback Method
tf	452.34	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.67	J/mol×K	716.17	Joback Method
cpg	565.39	J/mol×K	747.64	Joback Method
cpg	575.36	J/mol×K	779.12	Joback Method
cpg	584.61	J/mol×K	810.59	Joback Method
cpg	593.16	J/mol×K	842.07	Joback Method
cpg	601.02	J/mol×K	873.54	Joback Method
cpg	608.22	J/mol×K	905.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390854&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