Succinic acid, 2-chloro-6-fluorophenyl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C17H20ClFO4/c1-11-5-7-12(8-6-11)22-15(20)9-10-16(21)23-17-13(18)3-2-4-14

InchiKey: WJNVHCKAVKCFBU-UHFFFAOYSA-N

Formula: C17H20ClFO4

SMILES: CC1CCC(OC(=O)CCC(=O)Oc2c(F)cccc2Cl)CC1

Mol. weight [g/mol]: 342.79

Physical Properties

Property code	Value	Unit	Source
gf	-472.43	kJ/mol	Joback Method
hf	-848.09	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	79.04	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.287		Crippen Method
mcvol	244.660	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	829.16	K	Joback Method
tc	1051.23	K	Joback Method
tf	510.78	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.53	J/mol×K	829.16	Joback Method
cpg	750.68	J/mol×K	866.17	Joback Method
cpg	764.43	J/mol×K	903.18	Joback Method
cpg	776.80	J/mol×K	940.20	Joback Method
cpg	787.79	J/mol×K	977.21	Joback Method
cpg	797.42	J/mol×K	1014.22	Joback Method
cpg	805.69	J/mol×K	1051.23	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=U390059&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