Succinic acid, 2-chloro-6-fluorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H26ClFO4/c1-20(2,3)13-7-9-14(10-8-13)25-17(23)11-12-18(24)26-19-15(2

InchiKey: JPAVLEODQIKQRW-UHFFFAOYSA-N

Formula: C20H26ClFO4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)Oc2c(F)cccc2Cl)CC1

Mol. weight [g/mol]: 384.87

Physical Properties

Property code	Value	Unit	Source
gf	-444.33	kJ/mol	Joback Method
hf	-918.76	kJ/mol	Joback Method
hfus	39.16	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.313		Crippen Method
mcvol	286.930	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	894.57	K	Joback Method
tc	1119.30	K	Joback Method
tf	547.01	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.63	J/mol×K	894.57	Joback Method
cpg	926.01	J/mol×K	932.02	Joback Method
cpg	939.89	J/mol×K	969.48	Joback Method
cpg	952.31	J/mol×K	1006.93	Joback Method
cpg	963.32	J/mol×K	1044.39	Joback Method
cpg	972.95	J/mol×K	1081.84	Joback Method
cpg	981.25	J/mol×K	1119.30	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=U390201&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