Succinic acid, 2-chloro-6-fluorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C17H22ClFO4/c1-10(2)16(11(3)4)22-14(20)8-9-15(21)23-17-12(18)6-5-7-13(1
InchiKey: JLMAWKVGIYNTBP-UHFFFAOYSA-N
Formula: C17H22ClFO4
SMILES: CC(C)C(OC(=O)CCC(=O)Oc1c(F)cccc1Cl)C(C)C
Mol. weight [g/mol]: 344.81

Physical Properties

Property code	Value	Unit	Source
gf	-496.49	kJ/mol	Joback Method
hf	-897.91	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.388		Crippen Method
mcvol	255.520	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	812.96	K	Joback Method
tc	1019.90	K	Joback Method
tf	462.64	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.56	J/mol×K	812.96	Joback Method
cpg	753.74	J/mol×K	847.45	Joback Method
cpg	766.86	J/mol×K	881.94	Joback Method
cpg	778.90	J/mol×K	916.43	Joback Method
cpg	789.90	J/mol×K	950.92	Joback Method
cpg	799.86	J/mol×K	985.41	Joback Method
cpg	808.79	J/mol×K	1019.90	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=U390509&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