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

Inchi: InChI=1S/C18H16ClFO4/c1-11-5-3-8-15(12(11)2)23-16(21)9-10-17(22)24-18-13(19)6-4-
InchiKey: SXOVXROUFOQYIO-UHFFFAOYSA-N
Formula: C18H16ClFO4
SMILES: Cc1cccc(OC(=O)CCC(=O)Oc2c(F)cccc2Cl)c1C
Mol. weight [g/mol]: 350.77

Physical Properties

Property code	Value	Unit	Source
gf	-387.60	kJ/mol	Joback Method
hf	-689.12	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.387		Crippen Method
mcvol	245.850	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook
tb	873.80	K	Joback Method
tc	1100.20	K	Joback Method
tf	570.37	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.35	J/mol×K	873.80	Joback Method
cpg	706.12	J/mol×K	911.53	Joback Method
cpg	716.72	J/mol×K	949.27	Joback Method
cpg	726.15	J/mol×K	987.00	Joback Method
cpg	734.43	J/mol×K	1024.74	Joback Method
cpg	741.57	J/mol×K	1062.47	Joback Method
cpg	747.58	J/mol×K	1100.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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