Succinic acid, 2-chloro-6-fluorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C18H24ClFO4/c1-12(10-18(2,3)4)11-23-15(21)8-9-16(22)24-17-13(19)6-5-7-14

InchiKey: RYYFARZZBWEENM-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: CC(COC(=O)CCC(=O)Oc1c(F)cccc1Cl)CC(C)(C)C

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-480.35	kJ/mol	Joback Method
hf	-916.74	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.780		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	833.49	K	Joback Method
tc	1041.55	K	Joback Method
tf	506.33	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.72	J/mol×K	833.49	Joback Method
cpg	811.00	J/mol×K	868.17	Joback Method
cpg	824.20	J/mol×K	902.84	Joback Method
cpg	836.36	J/mol×K	937.52	Joback Method
cpg	847.51	J/mol×K	972.19	Joback Method
cpg	857.68	J/mol×K	1006.87	Joback Method
cpg	866.92	J/mol×K	1041.55	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=U389546&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