Succinic acid, 2-chloro-6-fluorophenyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C16H20ClFO4/c1-10(16(2,3)4)21-13(19)8-9-14(20)22-15-11(17)6-5-7-12(15)18

InchiKey: IYXMIUWMKIONOE-UHFFFAOYSA-N

Formula: C16H20ClFO4

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

Mol. weight [g/mol]: 330.78

Physical Properties

Property code	Value	Unit	Source
gf	-497.19	kJ/mol	Joback Method
hf	-875.46	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	75.01	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.142		Crippen Method
mcvol	241.430	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2039.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	787.73	K	Joback Method
tc	998.28	K	Joback Method
tf	483.79	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.20	J/mol×K	787.73	Joback Method
cpg	697.99	J/mol×K	822.82	Joback Method
cpg	710.76	J/mol×K	857.91	Joback Method
cpg	722.53	J/mol×K	893.01	Joback Method
cpg	733.33	J/mol×K	928.10	Joback Method
cpg	743.19	J/mol×K	963.19	Joback Method
cpg	752.15	J/mol×K	998.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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