2,6-Pyridinedicarboxylic acid, di(2-chloro-6-fluorophenyl) ester

Inchi: InChI=1S/C19H9Cl2F2NO4/c20-10-4-1-6-12(22)16(10)27-18(25)14-8-3-9-15(24-14)19(2

InchiKey: KSZMKMXQNPTBHM-UHFFFAOYSA-N

Formula: C19H9Cl2F2NO4

SMILES: O=C(Oc1c(F)cccc1Cl)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1

Mol. weight [g/mol]: 424.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	5.105		Crippen Method
mcvol	260.170	ml/mol	McGowan Method
rinpol	3010.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368989&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices