2,6-Pyridinedicarboxylic acid, butyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H15ClFNO4/c1-2-3-10-23-16(21)13-8-5-9-14(20-13)17(22)24-15-11(18)6-4

InchiKey: OHFBIYPMMOWPAX-UHFFFAOYSA-N

Formula: C17H15ClFNO4

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

Mol. weight [g/mol]: 351.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	4.050		Crippen Method
mcvol	241.740	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368980&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