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

Inchi: InChI=1S/C15H11ClFNO4/c1-2-21-14(19)11-7-4-8-12(18-11)15(20)22-13-9(16)5-3-6-10(

InchiKey: UGMBBZNFNHBSSA-UHFFFAOYSA-N

Formula: C15H11ClFNO4

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

Mol. weight [g/mol]: 323.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.270		Crippen Method
mcvol	213.560	ml/mol	McGowan Method
rinpol	2322.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368978&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices