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

Inchi: InChI=1S/C21H23ClFNO4/c1-2-3-4-5-6-7-14-27-20(25)17-12-9-13-18(24-17)21(26)28-19

InchiKey: GYRYPEFBNWMCDJ-UHFFFAOYSA-N

Formula: C21H23ClFNO4

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

Mol. weight [g/mol]: 407.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	5.611		Crippen Method
mcvol	298.100	ml/mol	McGowan Method
rinpol	2886.00		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=U368984&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