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

Inchi: InChI=1S/C24H29ClFNO4/c1-2-3-4-5-6-7-8-9-10-17-30-23(28)20-15-12-16-21(27-20)24(

InchiKey: MYMJMRARIHVJDL-UHFFFAOYSA-N

Formula: C24H29ClFNO4

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

Mol. weight [g/mol]: 449.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	6.781		Crippen Method
mcvol	340.370	ml/mol	McGowan Method
rinpol	3122.00		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=U368986&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