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

Inchi: InChI=1S/C25H31ClFNO4/c1-2-3-4-5-6-7-8-9-10-11-18-31-24(29)21-16-13-17-22(28-21)25(30)32-23-19(26)14-12-15-20(23)27/h12-17H,2-11,18H2,1H3

InchiKey: XXXYCTYLDQEYED-UHFFFAOYSA-N

Formula: C25H31ClFNO4

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

Mol. weight [g/mol]: 463.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.19		Crippen Method
logp	7.171		Crippen Method
mcvol	354.460	ml/mol	McGowan Method
rinpol	2186.00		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=U368987&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