

# 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(23)1  
**InchiKey:** MYMJMRARIHVJDL-UHFFFAOYSA-N  
**Formula:** C24H29ClFNO4  
**SMILES:** CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(F)ccc2Cl)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
rinpola	3122.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpola:** Non-polar retention indices

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