

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: GYRYPEFBNWCDJ-UHFFFAOYSA-N
Formula: C21H23ClFNO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2c(F)ccc2Cl)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
rinsol	2886.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
rinsol: Non-polar retention indices

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