

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

Inchi: InChI=1S/C15H11ClFNO4/c1-2-21-14(19)11-7-4-8-12(18-11)15(20)22-13-9(16)5-3-6-10(17)
InchiKey: UGMBBZNFNHBSSA-UHFFFAOYSA-N
Formula: C15H11ClFNO4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1
Mol. weight [g/mol]: 323.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.270		Crippen Method
mcvol	213.560	ml/mol	McGowan Method
rinpola	2322.00		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=U368978&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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