

2,6-Pyridinedicarboxylic acid, 2-chloro-6-fluorophenyl 2-methylhex-3-yl ester

InChI: InChI=1S/C20H21ClFNO4/c1-4-7-17(12(2)3)26-19(24)15-10-6-11-16(23-15)20(25)27-18
InChIKey: GYNARBVBPTWGSZ-UHFFFAOYSA-N
Formula: C20H21ClFNO4
SMILES: CCCC(OC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1)C(C)C
Mol. weight [g/mol]: 393.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.97		Crippen Method
logp	5.075		Crippen Method
mcvol	284.010	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368981&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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