

2,6-Pyridinedicarboxylic acid, di(2-chloro-6-fluorophenyl) ester

Inchi: InChI=1S/C19H9Cl2F2NO4/c20-10-4-1-6-12(22)16(10)27-18(25)14-8-3-9-15(24-14)19(21)1
InchiKey: KSZMKMXQNPTBHM-UHFFFAOYSA-N
Formula: C19H9Cl2F2NO4
SMILES: O=C(Oc1c(F)cccc1Cl)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1
Mol. weight [g/mol]: 424.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	5.105		Crippen Method
mcvol	260.170	ml/mol	McGowan Method
rinpola	3010.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368989&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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