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

Inchi: InChI=1S/C20H21ClFNO4/c1-2-3-4-5-6-13-26-19(24)16-11-8-12-17(23-16)20(25)27-18-1

InchiKey: NEIUMLQVRBMHBB-UHFFFAOYSA-N

Formula: C20H21ClFNO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1

Mol. weight [g/mol]: 393.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	5.220		Crippen Method
mcvol	284.010	ml/mol	McGowan Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U368983&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.