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

Inchi: InChI=1S/C23H27ClFNO4/c1-2-3-4-5-6-7-8-9-16-29-22(27)19-14-11-15-20(26-19)23(28)
InchiKey: LYANPBATKXPFDL-UHFFFAOYSA-N
Formula: C23H27ClFNO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1
Mol. weight [g/mol]: 435.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	6.391		Crippen Method
mcvol	326.280	ml/mol	McGowan Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook

Sources

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=U368985&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.