

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

Inchi: InChI=1S/C26H33ClFNO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-32-25(30)22-17-14-18-23(29-
InchiKey: CSSHGBYCNIWML-UHFFFAOYSA-N
Formula: C26H33ClFNO4
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1
Mol. weight [g/mol]: 478.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.61		Crippen Method
logp	7.561		Crippen Method
mcvol	368.550	ml/mol	McGowan Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		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=U368988&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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