

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

Inchi: InChI=1S/C19H19ClFNO4/c1-2-3-4-5-12-25-18(23)15-10-7-11-16(22-15)19(24)26-17-13
InchiKey: VJWCAUYOIIAIDF-UHFFFAOYSA-N
Formula: C19H19ClFNO4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2c(F)ccc2Cl)n1
Mol. weight [g/mol]: 379.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	4.830		Crippen Method
mcvol	269.920	ml/mol	McGowan Method
rinpola	2688.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368982&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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