

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

Inchi: InChI=1S/C17H15ClFNO4/c1-2-3-10-23-16(21)13-8-5-9-14(20-13)17(22)24-15-11(18)6-4
InchiKey: OHFBIYPMOWPAX-UHFFFAOYSA-N
Formula: C17H15ClFNO4
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2c(F)cccc2Cl)n1
Mol. weight [g/mol]: 351.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	4.050		Crippen Method
mcvol	241.740	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368980&Units=SI>
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>

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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