2,6-Pyridinedicarboxylic acid, isopropyl pentyl ester

Inchi: InChI=1S/C15H21NO4/c1-4-5-6-10-19-14(17)12-8-7-9-13(16-12)15(18)20-11(2)3/h7-9,1

InchiKey: SNUJIVZGPNGXMP-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OC(C)C)n1

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	2.994		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpol	1998.00		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=U369149&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

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