2,6-Pyridinedicarboxylic acid, ethyl 2-pentyl ester

Inchi: InChI=1S/C14H19NO4/c1-4-7-10(3)19-14(17)12-9-6-8-11(15-12)13(16)18-5-2/h6,8-10H,

InchiKey: OXDFZVQNVWAHOY-UHFFFAOYSA-N

Formula: C14H19NO4

SMILES: CCCC(C)OC(=O)c1cccc(C(=O)OCC)n1

Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.604		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinpol	1882.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368332&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

rinpol: Non-polar retention indices