2,6-Pyridinedicarboxylic acid, 1-methoxydec-4-yl propyl ester

Inchi: InChI=1S/C21H33NO5/c1-4-6-7-8-11-17(12-10-16-25-3)27-21(24)19-14-9-13-18(22-19)2

InchiKey: JVTCWGVGMZQNSU-UHFFFAOYSA-N

Formula: C21H33NO5

SMILES: CCCCCCC(CCCOC)OC(=O)c1cccc(C(=O)OCCC)n1

Mol. weight [g/mol]: 379.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.94		Crippen Method
logp	4.571		Crippen Method
mcvol	313.720	ml/mol	McGowan Method
rinpol	2587.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369243&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

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