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

Inchi: InChI=1S/C23H37NO5/c1-4-6-8-9-13-19(14-12-17-27-3)29-23(26)21-16-11-15-20(24-21)22(25)28-18-10-7-5-2/h11,15-16,19H,4-10,12-14,17-18H2,1-3H3

InchiKey: RDFMTODMBGLODG-UHFFFAOYSA-N

Formula: C23H37NO5

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

Mol. weight [g/mol]: 407.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	5.351		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
rinpol	2769.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369246&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