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

Inchi: InChI=1S/C24H39NO5/c1-4-6-8-10-14-20(15-13-18-28-3)30-24(27)22-17-12-16-21(25-22

InchiKey: MXYWWINIQZFMLM-UHFFFAOYSA-N

Formula: C24H39NO5

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(CCCCCC)CCCOC)n1

Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	5.741		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
rinpol	2859.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369247&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices