2,6-Pyridinedicarboxylic acid, di(1-methoxydec-4-yl) ester

Inchi: InChI=1S/C29H49NO6/c1-5-7-9-11-16-24(18-14-22-33-3)35-28(31)26-20-13-21-27(30-26

InchiKey: IZAQUAZISDALES-UHFFFAOYSA-N

Formula: C29H49NO6

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

Mol. weight [g/mol]: 507.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	6.926		Crippen Method
mcvol	432.310	ml/mol	McGowan Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		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=U369253&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.