2,6-Pyridinedicarboxylic acid, 5-methoxy-3-methylpent-2-yl tetradecyl ester

Inchi: InChI=1S/C28H47NO5/c1-5-6-7-8-9-10-11-12-13-14-15-16-21-33-27(30)25-18-17-19-26(

InchiKey: ZGGFTPWVOHULRM-UHFFFAOYSA-N

Formula: C28H47NO5

SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1

Mol. weight [g/mol]: 477.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.63		Crippen Method
logp	7.157		Crippen Method
mcvol	412.350	ml/mol	McGowan Method
rinpol	3198.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369180&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