2,6-Pyridinedicarboxylic acid, 3-methylbutyl undecyl ester

Inchi: InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-17-27-22(25)20-14-13-15-21(24-20)23(2

InchiKey: BWUQYCJPBKOVMR-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	5.972		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2808.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368323&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