2,6-Pyridinedicarboxylic acid, isobutyl 3-(2-methoxyethyl)nonyl ester

Inchi: InChI=1S/C23H37NO5/c1-5-6-7-8-10-19(13-15-27-4)14-16-28-22(25)20-11-9-12-21(24-2

InchiKey: HGAKBZYQASXDOR-UHFFFAOYSA-N

Formula: C23H37NO5

SMILES: CCCCCCC(CCOC)CCOC(=O)c1cccc(C(=O)OCC(C)C)n1

Mol. weight [g/mol]: 407.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	5.064		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
rinpol	2795.00		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=U369207&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