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

Inchi: InChI=1S/C31H53NO6/c1-5-7-9-11-14-26(18-22-35-3)20-24-37-30(33)28-16-13-17-29(32

InchiKey: NKGUMMSUBQJIJS-UHFFFAOYSA-N

Formula: C31H53NO6

SMILES: CCCCCCC(CCOC)CCOC(=O)c1cccc(C(=O)OCCC(CCCCCC)CCOC)n1

Mol. weight [g/mol]: 535.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.62		Crippen Method
logp	7.422		Crippen Method
mcvol	460.490	ml/mol	McGowan Method
rinpol	3456.00		NIST Webbook
rinpol	3456.00		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=U369213&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.