2,6-Pyridinedicarboxylic acid, dodecyl 2-(2-methoxyethyl)heptyl ester

Inchi: InChI=1S/C29H49NO5/c1-4-6-8-9-10-11-12-13-14-16-22-34-28(31)26-19-17-20-27(30-26

InchiKey: YPJOIZWXILBDID-UHFFFAOYSA-N

Formula: C29H49NO5

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(CCCCC)CCOC)n1

Mol. weight [g/mol]: 491.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	7.549		Crippen Method
mcvol	426.440	ml/mol	McGowan Method
rinpol	3251.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369192&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