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

Inchi: InChI=1S/C24H39NO5/c1-4-6-8-9-11-17-29-23(26)21-14-12-15-22(25-21)24(27)30-19-20

InchiKey: DKOGNVMTSZOSEX-UHFFFAOYSA-N

Formula: C24H39NO5

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

Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	5.599		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
rinpol	2918.00		NIST Webbook

Sources

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=U369188&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices