2,6-Pyridinedicarboxylic acid, 3-(2-methoxyethyl)heptyl pentyl ester

Inchi: InChI=1S/C22H35NO5/c1-4-6-8-15-27-21(24)19-11-9-12-20(23-19)22(25)28-17-14-18(10

InchiKey: JBUUCRINRSURFK-UHFFFAOYSA-N

Formula: C22H35NO5

SMILES: CCCCCOC(=O)c1cccc(C(=O)OCCC(CCCC)CCOC)n1

Mol. weight [g/mol]: 393.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	4.818		Crippen Method
mcvol	327.810	ml/mol	McGowan Method
rinpol	2764.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369113&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices