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

Inchi: InChI=1S/C26H43NO5/c1-4-6-8-10-12-19-31-25(28)23-15-13-16-24(27-23)26(29)32-21-1

InchiKey: PRPLEHJBHVEKMJ-UHFFFAOYSA-N

Formula: C26H43NO5

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

Mol. weight [g/mol]: 449.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	6.379		Crippen Method
mcvol	384.170	ml/mol	McGowan Method
rinpol	3078.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369211&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