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

Inchi: InChI=1S/C27H45NO6/c1-5-7-9-12-22(16-18-31-3)20-33-26(29)24-14-11-15-25(28-24)27

InchiKey: WRGRSECEIWPOMB-UHFFFAOYSA-N

Formula: C27H45NO6

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

Mol. weight [g/mol]: 479.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.95		Crippen Method
logp	5.861		Crippen Method
mcvol	404.130	ml/mol	McGowan Method
rinpol	3127.00		NIST Webbook
rinpol	3127.00		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=U369193&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.