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

Inchi: InChI=1S/C19H29NO5/c1-4-6-8-15(11-13-23-3)12-14-25-19(22)17-10-7-9-16(20-17)18(2

InchiKey: FPHUVROUQOWHPD-UHFFFAOYSA-N

Formula: C19H29NO5

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

Mol. weight [g/mol]: 351.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	3.648		Crippen Method
mcvol	285.540	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369110&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

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