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

Inchi: InChI=1S/C25H41NO5/c1-4-6-8-9-10-11-18-30-24(27)22-14-12-15-23(26-22)25(28)31-20

InchiKey: HPMSOSYNLACFEX-UHFFFAOYSA-N

Formula: C25H41NO5

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

Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.27		Crippen Method
logp	5.989		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
rinpol	3017.00		NIST Webbook
rinpol	3017.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369116&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

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