2,6-Pyridinedicarboxylic acid, decyl dodecyl ester

Inchi: InChI=1S/C29H49NO4/c1-3-5-7-9-11-13-14-16-18-20-25-34-29(32)27-23-21-22-26(30-27

InchiKey: HZRZHFRSWXNYCY-UHFFFAOYSA-N

Formula: C29H49NO4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCC)n1

Mol. weight [g/mol]: 475.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.09		Crippen Method
logp	8.457		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368814&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/48-447-3/2-6-Pyridinedicarboxylic-acid-decyl-dodecyl-ester.pdf
Generated by Cheméo on 2024-04-29 13:10:27.964385792 +0000 UTC m=+16685476.884963104.

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