2,6-Pyridinedicarboxylic acid, 2,4,4-trimethylpentyl undecyl ester

Inchi: InChI=1S/C26H43NO4/c1-6-7-8-9-10-11-12-13-14-18-30-24(28)22-16-15-17-23(27-22)25

InchiKey: GTYCLSGLKYYSLP-UHFFFAOYSA-N

Formula: C26H43NO4

SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1

Mol. weight [g/mol]: 433.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.36		Crippen Method
logp	6.998		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		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=U368797&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

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