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

Inchi: InChI=1S/C29H49NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-21-33-27(31)25-19-18-20-26

InchiKey: SJQLECJVTMNGLQ-UHFFFAOYSA-N

Formula: C29H49NO4

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

Mol. weight [g/mol]: 475.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.61		Crippen Method
logp	8.169		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		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=U368800&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.