2,6-Pyridinedicarboxylic acid, heptadecyl neopentyl ester

Inchi: InChI=1S/C29H49NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-33-27(31)25-21-

InchiKey: VVNGVGKCASZOQM-UHFFFAOYSA-N

Formula: C29H49NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1

Mol. weight [g/mol]: 475.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.85		Crippen Method
logp	8.313		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3207.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369013&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