2,6-Pyridinedicarboxylic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C23H37NO4/c1-16(12-22(3,4)5)14-27-20(25)18-10-9-11-19(24-18)21(26)28-15-17(2)13-23(6,7)8/h9-11,16-17H,12-15H2,1-8H3

InchiKey: CJIGHZBOSRMTMZ-UHFFFAOYSA-N

Formula: C23H37NO4

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

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	5.540		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2529.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368805&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices