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

Inchi: InChI=1S/C23H37NO4/c1-6-7-8-9-10-11-15-27-21(25)19-13-12-14-20(24-19)22(26)28-17

InchiKey: LGQJZJZBUWRWNP-UHFFFAOYSA-N

Formula: C23H37NO4

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

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.828		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2665.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368794&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