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

Inchi: InChI=1S/C19H29NO4/c1-6-7-11-23-17(21)15-9-8-10-16(20-15)18(22)24-13-14(2)12-19(

InchiKey: VOSPWLIGKYJUAB-UHFFFAOYSA-N

Formula: C19H29NO4

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

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.268		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2279.00		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=U368790&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

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