

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

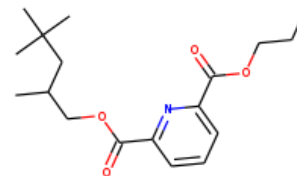
InChI: InChI=1S/C18H27NO4/c1-6-10-22-16(20)14-8-7-9-15(19-14)17(21)23-12-13(2)11-18(3,4)5/h7-9,13H,6,10-12H2,1-5H3

InChI Key: NJVRBVJVODBHAF-UHFFFAOYSA-N

Formula: C18H27NO4

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

Molecular Weight: 321.41



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.878		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H27NO4/c1-6-10-22-16\(20\)14-8-7-9-15\(19-14\)17\(21\)23-12-13\(2\)11-18\(3,4\)5/h7-9,13H,6,10-12H2,1-5H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H27NO4/c1-6-10-22-16(20)14-8-7-9-15(19-14)17(21)23-12-13(2)11-18(3,4)5/h7-9,13H,6,10-12H2,1-5H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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