# 2,6-Pyridinedicarboxylic acid, 2-methylhex-3-yl 2,4,4-trimethylpentyl ester

**Inchi:** InChI=1S/C22H35NO4/c1-8-10-19(15(2)3)27-21(25)18-12-9-11-17(23-18)20(24)26-14-16

**InchiKey:** BNGFULGSXWTPID-UHFFFAOYSA-N

**Formula:** C22H35NO4

**SMILES:** CCCC(OC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1)C(C)C

**Mol. weight [g/mol]:** 377.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.55 | | Crippen Method |
| logp | 5.292 | | Crippen Method |
| mcvol | 321.940 | ml/mol | McGowan Method |
| rinpol | 2396.00 | | 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=U368792&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