# 2,6-Pyridinedicarboxylic acid, hexyl undecyl ester

**Inchi:** InChI=1S/C24H39NO4/c1-3-5-7-9-10-11-12-13-15-20-29-24(27)22-18-16-17-21(25-22)23

**InchiKey:** IYBHGUFZDFXOPD-UHFFFAOYSA-N

**Formula:** C24H39NO4

**SMILES:** CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCC)n1

**Mol. weight [g/mol]:** 405.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -8.00 | | Crippen Method |
| logp | 6.506 | | Crippen Method |
| mcvol | 350.120 | ml/mol | McGowan Method |
| rinpol | 2933.00 | | NIST Webbook |
| rinpol | 2933.00 | | NIST Webbook |

## Sources

**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=U368779&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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