# 2,6-Pyridinedicarboxylic acid, dodecyl neopentyl ester

**Inchi:** InChI=1S/C24H39NO4/c1-5-6-7-8-9-10-11-12-13-14-18-28-22(26)20-16-15-17-21(25-20)
**InchiKey:** SQDSEPXNXSAIEE-UHFFFAOYSA-N
**Formula:** C24H39NO4
**SMILES:** CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
**Mol. weight [g/mol]:** 405.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.76 | | Crippen Method |
| logp | 6.362 | | Crippen Method |
| mcvol | 350.120 | ml/mol | McGowan Method |
| rinpol | 2819.00 | | NIST Webbook |
| rinpol | 2819.00 | | 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=U369008&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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