# Isonipecotic acid, N-methoxycarbonyl-, undecyl ester

**Inchi:** InChI=1S/C19H35NO4/c1-3-4-5-6-7-8-9-10-11-16-24-18(21)17-12-14-20(15-13-17)19(22

**InchiKey:** XAOWQIOAXUQFCW-UHFFFAOYSA-N

**Formula:** C19H35NO4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1

**Mol. weight [g/mol]:** 341.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.70 | | Crippen Method |
| logp | 4.539 | | Crippen Method |
| mcvol | 292.570 | ml/mol | McGowan Method |
| rinpol | 2526.00 | | NIST Webbook |
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## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U322027&Units=SI

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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## 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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