# Pipecolic acid, N-octyloxycarbonyl-, undecyl ester

**Inchi:** InChI=1S/C26H49NO4/c1-3-5-7-9-11-12-13-15-18-22-30-25(28)24-20-16-17-21-27(24)26

**InchiKey:** PTSSMXITPGQEHQ-UHFFFAOYSA-N

**Formula:** C26H49NO4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCCCCCCCC

**Mol. weight [g/mol]:** 439.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.99 | | Crippen Method |
| logp | 7.412 | | Crippen Method |
| mcvol | 391.200 | ml/mol | McGowan Method |
| rinpol | 3045.00 | | NIST Webbook |
| rinpol | 3045.00 | | NIST Webbook |

## Sources

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U393132&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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