

# Isonipecotic acid, N-(3-methoxybenzoyl)-, undecyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C25H39NO4/c1-3-4-5-6-7-8-9-10-11-19-30-25(28)21-15-17-26(18-16-21)24(27) |
| InchiKey:            | SMISCKNWQLDRLF-UHFFFAOYSA-N   |
| Formula:             | C25H39NO4   |
| SMILES:              | CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(OC)c2)CC1   |
| Mol. weight [g/mol]: | 417.58  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.53   |        | Crippen Method |
| logp          | 5.621   |        | Crippen Method |
| mcvol         | 353.350 | ml/mol | McGowan Method |
| rinpol        | 3447.00 |        | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361183&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361183&amp;Units=SI</a> |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |
| rinpol:  | Non-polar retention indices         |

Latest version available from:

<https://www.chemeo.com/cid/56-901-9/Isonipecotic-acid-N-3-methoxybenzoyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 10:40:49.43656787 +0000 UTC m=+16158098.357145183.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.