# Isonipecotic acid, N-(3-methylbenzoyl)-, pentyl ester

**Inchi:** InChI=1S/C19H27NO3/c1-3-4-5-13-23-19(22)16-9-11-20(12-10-16)18(21)17-8-6-7-15(2)

**InchiKey:** UZMBVCWEXGAODT-UHFFFAOYSA-N

**Formula:** C19H27NO3

**SMILES:** CCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1

**Mol. weight [g/mol]:** 317.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.37 | | Crippen Method |
| logp | 3.581 | | Crippen Method |
| mcvol | 262.940 | ml/mol | McGowan Method |
| rinpol | 2654.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U361099&Units=SI

**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

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices