# Isonipecotic acid, N-pentafluorobenzoyl-, ethyl ester

**Inchi:** InChI=1S/C15H14F5NO3/c1-2-24-15(23)7-3-5-21(6-4-7)14(22)8-9(16)11(18)13(20)12(19

**InchiKey:** UNCLJTXXIGBVMY-UHFFFAOYSA-N

**Formula:** C15H14F5NO3

**SMILES:** CCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1

**Mol. weight [g/mol]:** 351.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.30 | | Crippen Method |
| logp | 2.797 | | Crippen Method |
| mcvol | 215.430 | ml/mol | McGowan Method |
| rinpol | 2004.00 | | 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=U361220&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