# Isonipecotic acid, N-pentafluorobenzoyl-, propyl ester

**Inchi:** InChI=1S/C16H16F5NO3/c1-2-7-25-16(24)8-3-5-22(6-4-8)15(23)9-10(17)12(19)14(21)13

**InchiKey:** TZNALVRMLVELHJ-UHFFFAOYSA-N

**Formula:** C16H16F5NO3

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

**Mol. weight [g/mol]:** 365.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.72 | | Crippen Method |
| logp | 3.188 | | Crippen Method |
| mcvol | 229.520 | ml/mol | McGowan Method |
| rinpol | 2107.00 | | NIST Webbook |
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## 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=U361221&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

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