

# Isonipecotic acid, N-benzoyl-, propyl ester

**Inchi:** InChI=1S/C16H21NO3/c1-2-12-20-16(19)14-8-10-17(11-9-14)15(18)13-6-4-3-5-7-13/h3-  
**InchiKey:** JUEQUPTYGYSLEP-UHFFFAOYSA-N  
**Formula:** C16H21NO3  
**SMILES:** CCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1  
**Mol. weight [g/mol]:** 275.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.492		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U360971&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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