

# Isonipecotic acid, N-benzoyl-, heptyl ester

**Inchi:** InChI=1S/C20H29NO3/c1-2-3-4-5-9-16-24-20(23)18-12-14-21(15-13-18)19(22)17-10-7-6  
**InchiKey:** KBOYYWPLMVQSAJ-UHFFFAOYSA-N  
**Formula:** C20H29NO3  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1  
**Mol. weight [g/mol]:** 331.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	4.052		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpole	2767.00		NIST Webbook
rinpole	2767.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360977&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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