

# Isonipecotic acid, N-(3-phenylpropionyl)-, butyl ester

**Inchi:** InChI=1S/C19H27NO3/c1-2-3-15-23-19(22)17-11-13-20(14-12-17)18(21)10-9-16-7-5-4-6  
**InchiKey:** LMNVCCRMMGJHOW-UHFFFAOYSA-N  
**Formula:** C19H27NO3  
**SMILES:** CCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1  
**Mol. weight [g/mol]:** 317.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	3.201		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2679.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=U361557&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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