

# Isonipectic acid, N-benzoyl-, butyl ester

**Inchi:** InChI=1S/C17H23NO3/c1-2-3-13-21-17(20)15-9-11-18(12-10-15)16(19)14-7-5-4-6-8-14/  
**InchiKey:** XDSIJHWAZYZQKO-UHFFFAOYSA-N  
**Formula:** C17H23NO3  
**SMILES:** CCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1  
**Mol. weight [g/mol]:** 289.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.882		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rmpol	2462.00		NIST Webbook
rmpol	2462.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360973&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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