

# Isonipecotic acid, n-butoxycarbonyl-, pentyl ester

**Inchi:** InChI=1S/C16H29NO4/c1-3-5-7-13-20-15(18)14-8-10-17(11-9-14)16(19)21-12-6-4-2/h14  
**InchiKey:** DEUNKXRGRYEBHV-UHFFFAOYSA-N  
**Formula:** C16H29NO4  
**SMILES:** CCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1  
**Mol. weight [g/mol]:** 299.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	3.368		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rmpol	2171.00		NIST Webbook
rmpol	2171.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322049&Units=SI>

## 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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