

# Isonipecotic acid, N-allyloxycarbonyl-, octyl ester

**Inchi:** InChI=1S/C18H31NO4/c1-3-5-6-7-8-9-15-22-17(20)16-10-12-19(13-11-16)18(21)23-14-4  
**InchiKey:** AFRCDGZDCUWFRR-UHFFFAOYSA-N  
**Formula:** C18H31NO4  
**SMILES:** C=CCOC(=O)N1CCC(C(=O)OCCCCCCCC)CC1  
**Mol. weight [g/mol]:** 325.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	3.925		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
rmpol	2361.00		NIST Webbook
rmpol	2361.00		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=U321995&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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