

# Isonipecotic acid, N-(octanoyl)-, pentyl ester

**Inchi:** InChI=1S/C19H35NO3/c1-3-5-7-8-9-11-18(21)20-14-12-17(13-15-20)19(22)23-16-10-6-4  
**InchiKey:** MLTXTFKFLZMCRQ-UHFFFAOYSA-N  
**Formula:** C19H35NO3  
**SMILES:** CCCCCC(=O)N1CCC(C(=O)OCCCC)CC1  
**Mol. weight [g/mol]:** 325.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.319		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
rmpol	2563.00		NIST Webbook
rmpol	2563.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361570&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  
**rmpol:** Non-polar retention indices

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