

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

**Inchi:** InChI=1S/C18H33NO3/c1-3-5-7-8-9-10-17(20)19-13-11-16(12-14-19)18(21)22-15-6-4-2/  
**InchiKey:** ZJAZLRTWQAOHLI-UHFFFAOYSA-N  
**Formula:** C18H33NO3  
**SMILES:** CCCCCC(=O)N1CCC(C(=O)OCCCC)CC1  
**Mol. weight [g/mol]:** 311.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	3.929		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
rinpola	2460.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361569&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/17-696-1/Isonipecotic-acid-N-octanoyl-butyl-ester.pdf>

Generated by Cheméo on 2024-04-23 16:13:55.780148356 +0000 UTC m=+16178084.700725668.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.