

# Isonipectic acid, N-isobutoxycarbonyl-, octyl ester

**Inchi:** InChI=1S/C19H35NO4/c1-4-5-6-7-8-9-14-23-18(21)17-10-12-20(13-11-17)19(22)24-15-1  
**InchiKey:** LIAUYFRERHMYRY-UHFFFAOYSA-N  
**Formula:** C19H35NO4  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1  
**Mol. weight [g/mol]:** 341.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	4.395		Crippen Method
mcvol	292.570	ml/mol	McGowan Method

## 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=U322067&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/99-642-0/Isonipectic-acid-N-isobutoxycarbonyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-23 06:25:13.169886414 +0000 UTC m=+16142762.090463729.

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