

# Isonipectic acid, N-(cyclohexylcarbonyl)-, octyl ester

**Inchi:** InChI=1S/C21H37NO3/c1-2-3-4-5-6-10-17-25-21(24)19-13-15-22(16-14-19)20(23)18-11-12  
**InchiKey:** UBVLQYGIOIWR-UHFFFAOYSA-N  
**Formula:** C<sub>21</sub>H<sub>37</sub>NO<sub>3</sub>  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1  
**Mol. weight [g/mol]:** 351.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.709		Crippen Method
mcvol	304.020	ml/mol	McGowan Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361031&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  
**rinpol:** Non-polar retention indices

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