

# Isonipecotic acid, N-(2-furoyl)-, octyl ester

**Inchi:** InChI=1S/C19H29NO4/c1-2-3-4-5-6-7-14-24-19(22)16-10-12-20(13-11-16)18(21)17-9-8-  
**InchiKey:** DLUBDUXNJOMYRN-UHFFFAOYSA-N  
**Formula:** C19H29NO4  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1  
**Mol. weight [g/mol]:** 335.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.89		Crippen Method
logp	4.036		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361506&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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