

# Isonipecotic acid, N-(2-methoxybenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C20H29NO4/c1-3-4-5-8-15-25-20(23)16-11-13-21(14-12-16)19(22)17-9-6-7-10  
**InchiKey:** ZXDZWBBICBYWFO-UHFFFAOYSA-N  
**Formula:** C20H29NO4  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1  
**Mol. weight [g/mol]:** 347.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.671		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
rinpola	2797.00		NIST Webbook
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## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361190&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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