

# Isonipecotic acid, N-(3-methoxybenzoyl)-, hexyl ester

<b>Inchi:</b>	InChI=1S/C20H29NO4/c1-3-4-5-6-14-25-20(23)16-10-12-21(13-11-16)19(22)17-8-7-9-18
<b>InchiKey:</b>	HHMDRIKBJAIMJT-UHFFFAOYSA-N
<b>Formula:</b>	C20H29NO4
<b>SMILES:</b>	CCCCCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)CC1
<b>Mol. weight [g/mol]:</b>	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
rinpole	2906.00		NIST Webbook
rinpole	2906.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361178&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361178&amp;Units=SI</a>

## Legend

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

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