

# Isonipecotic acid, N-(4-butylbenzoyl)-, octyl ester

<b>Inchi:</b>	InChI=1S/C25H39NO3/c1-3-5-7-8-9-10-20-29-25(28)23-16-18-26(19-17-23)24(27)22-14
<b>InchiKey:</b>	VOMLUEQYWMGTFQ-UHFFFAOYSA-N
<b>Formula:</b>	C25H39NO3
<b>SMILES:</b>	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(CCCC)cc2)CC1
<b>Mol. weight [g/mol]:</b>	401.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	5.785		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
rinsol	3323.00		NIST Webbook
rinsol	3323.00		NIST Webbook

## Sources

<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=U361135&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361135&amp;Units=SI</a>
<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>

## 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>rinsol:</b>	Non-polar retention indices

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