

# Isonipecotic acid, N-(3-methylbenzoyl)-, dodecyl ester

<b>Inchi:</b>	InChI=1S/C26H41NO3/c1-3-4-5-6-7-8-9-10-11-12-20-30-26(29)23-16-18-27(19-17-23)25
<b>InchiKey:</b>	DAKOUQRWGYDLTR-UHFFFAOYSA-N
<b>Formula:</b>	C26H41NO3
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1
<b>Mol. weight [g/mol]:</b>	415.61

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	6.311		Crippen Method
mcvol	361.570	ml/mol	McGowan Method
rinpola	3403.00		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=U361107&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361107&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>rinpola:</b>	Non-polar retention indices

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