

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

<b>Inchi:</b>	InChI=1S/C26H41NO4/c1-3-4-5-6-7-8-9-10-11-14-21-31-26(29)22-17-19-27(20-18-22)25
<b>InchiKey:</b>	WVOVFNHPUONTAI-UHFFFAOYSA-N
<b>Formula:</b>	C26H41NO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
<b>Mol. weight [g/mol]:</b>	431.61

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.95		Crippen Method
logp	6.011		Crippen Method
mcvol	367.440	ml/mol	McGowan Method
rinpola	3447.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U361196&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361196&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>

## 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

Latest version available from:

<https://www.chemeo.com/cid/32-054-6/Isonipecotic-acid-N-2-methoxybenzoyl-dodecyl-ester.pdf>

Generated by Cheméo on 2024-04-27 14:59:01.989532313 +0000 UTC m=+16519190.910109627.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.