

# Isonipecotic acid, N-methoxycarbonyl-, heptadecyl ester

<b>Inchi:</b>	InChI=1S/C25H47NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-30-24(27)23-18-20
<b>InchiKey:</b>	AQQAQOYZFTCDFNT-UHFFFAOYSA-N
<b>Formula:</b>	C25H47NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
<b>Mol. weight [g/mol]:</b>	425.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	6.879		Crippen Method
mcvol	377.110	ml/mol	McGowan Method

## 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=U322032&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322032&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>

## 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

Latest version available from:

<https://www.chemeo.com/cid/83-914-5/Isonipecotic-acid-N-methoxycarbonyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2024-04-28 06:11:01.479596989 +0000 UTC m=+16573910.400174317.

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