

# Isonicotinic acid, 4-tetradecyl ester

<b>Inchi:</b>	InChI=1S/C20H33NO2/c1-3-5-6-7-8-9-10-11-13-19(12-4-2)23-20(22)18-14-16-21-17-15-
<b>InchiKey:</b>	GNAGQRKHMNLHHW-UHFFFAOYSA-N
<b>Formula:</b>	C20H33NO2
<b>SMILES:</b>	CCCCCCCCCCC(CCC)OC(=O)c1ccncc1
<b>Mol. weight [g/mol]:</b>	319.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.938		Crippen Method
mcvol	286.320	ml/mol	McGowan Method

## 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.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=U299899&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299899&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

Latest version available from:

<https://www.chemeo.com/cid/98-074-2/Isonicotinic-acid-4-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-19 15:47:46.880271708 +0000 UTC m=+15830915.800849024.

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