

# Pyridine-2-carboxylic acid, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C20H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-23-20(22)19-16-13-14-17-21-
<b>InchiKey:</b>	XYCRWADEMHQUCD-UHFFFAOYSA-N
<b>Formula:</b>	C20H33NO2
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1ccccn1
<b>Mol. weight [g/mol]:</b>	319.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.92		Crippen Method
logp	5.939		Crippen Method
mcvol	286.320	ml/mol	McGowan Method
rinpol	2508.00		NIST Webbook

## 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=U369166&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369166&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
<b>rinpol:</b>	Non-polar retention indices

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