

# Isonicotinic acid, 2-pentadecyl ester

<b>Inchi:</b>	InChI=1S/C21H35NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-19(2)24-21(23)20-15-17-22-18-
<b>InchiKey:</b>	YMMYDCKSIRLPIH-UHFFFAOYSA-N
<b>Formula:</b>	C21H35NO2
<b>SMILES:</b>	CCCCCCCCCCCC(C)OC(=O)c1ccncc1
<b>Mol. weight [g/mol]:</b>	333.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	6.328		Crippen Method
mcvol	300.410	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=U299901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299901&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

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