

# Octyl nicotinate

<b>Other names:</b>	Nicotinic acid, octyl ester
<b>Inchi:</b>	InChI=1S/C14H21NO2/c1-2-3-4-5-6-7-11-17-14(16)13-9-8-10-15-12-13/h8-10,12H,2-7,1
<b>InchiKey:</b>	TYBQVEHLLOHMLT-UHFFFAOYSA-N
<b>Formula:</b>	C14H21NO2
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccnc1
<b>Mol. weight [g/mol]:</b>	235.32
<b>CAS:</b>	40975-41-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.599		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
rmpol	1800.00		NIST Webbook
rmpol	1800.00		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=C40975415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40975415&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
<b>rmpol:</b>	Non-polar retention indices

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