

# Isonicotinic acid, 2-tetrahydrofurylmethyl ester

<b>Inchi:</b>	InChI=1S/C11H13NO3/c13-11(9-3-5-12-6-4-9)15-8-10-2-1-7-14-10/h3-6,10H,1-2,7-8H2
<b>InchiKey:</b>	UALDAZFAVQFVDG-UHFFFAOYSA-N
<b>Formula:</b>	C11H13NO3
<b>SMILES:</b>	O=C(OCC1CCCO1)c1ccncc1
<b>Mol. weight [g/mol]:</b>	207.23

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.417		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
rinsol	1648.00		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=U308336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308336&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>rinsol:</b>	Non-polar retention indices

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