

# Isopropyl nicotinate

<b>Other names:</b>	3-Pyridinecarboxylic acid, 1-methylethyl ester Nicotinic acid, isopropyl ester Nipyl
<b>Inchi:</b>	InChI=1S/C9H11NO2/c1-7(2)12-9(11)8-4-3-5-10-6-8/h3-7H,1-2H3
<b>InchiKey:</b>	VSRSQDMWBSKNSF-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO2
<b>SMILES:</b>	CC(C)OC(=O)c1cccnc1
<b>Mol. weight [g/mol]:</b>	165.19
<b>CAS:</b>	553-60-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	1.647		Crippen Method
mcvol	131.330	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.20	K	4.00	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=C553606&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C553606&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>tbrp:</b>	Boiling point at reduced pressure

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