

# 3-Pyridinecarboxaldehyde

<b>Other names:</b>	Nicotinaldehyde «beta»-Pyridinecarbaldehyde Nicotinealdehyde Nicotinic aldehyde Rowalind 3-Formylpyridine 3-Pyridinaldehyde 3-Pyridinealdehyde 3-Pyridylaldehyde 3-Pyridylcarboxaldehyde 3-Nicotinaldehyde Pyridine-3-carboxaldehyde Pyridine-3-aldehyde 3-Pyridinecarbaldehyde Pyridine-3-carbaldehyde NSC 8952
<b>Inchi:</b>	InChI=1S/C6H5NO/c8-5-6-2-1-3-7-4-6/h1-5H
<b>InchiKey:</b>	QJZUKDFHGGYHMC-UHFFFAOYSA-N
<b>Formula:</b>	C6H5NO
<b>SMILES:</b>	O=Cc1cccnc1
<b>Mol. weight [g/mol]:</b>	107.11
<b>CAS:</b>	500-22-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	0.894		Crippen Method
mcvol	83.190	ml/mol	McGowan Method
rinpol	968.00		NIST Webbook
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## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	2.00	NIST Webbook

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## Sources

<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=C500221&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C500221&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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
<b>tbrp:</b>	Boiling point at reduced pressure

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