

# Nicotinyl alcohol

<b>Other names:</b>	.beta.-picolyl alcohol 3-(Hydroxymethyl)pyridine 3-Pyridinemethanol 3-Pyridinylmethanol 3-Pyridylcarbinol 3-Pyridylmethanol 3-hydroxymethylpyridine NSC 526046 Nicotinic alcohol Niltuvin (free base) Nu-2121 Pyridine-3-carbinol Pyridine-3-methanol Pyridyl-3-carbinol Pyridyl-3-methanol RO-1-5155 Roniacol pyridine, 3-hydroxymethyl- «beta»-Picolyl alcohol «beta»-Pyridinecarbinol «beta»-Pyridylcarbinol Â«betaÂ»-Picolyl alcohol Â«betaÂ»-Pyridinecarbinol Â«betaÂ»-Pyridylcarbinol
<b>Inchi:</b>	InChI=1S/C6H7NO/c8-5-6-2-1-3-7-4-6/h1-4,8H,5H2
<b>InchiKey:</b>	MVQVNTPHUGQQHK-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO
<b>SMILES:</b>	OCc1cccnc1
<b>Mol. weight [g/mol]:</b>	109.13
<b>CAS:</b>	100-55-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.96		Aqueous Solubility Prediction Method
logp	0.574		Crippen Method
mvol	87.490	ml/mol	McGowan Method

rinpol	1119.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tf	266.40	K	Aqueous Solubility Prediction Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhoI	1138.20	kg/m <sup>3</sup>	291.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1137.50	kg/m <sup>3</sup>	292.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1136.80	kg/m <sup>3</sup>	293.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1135.30	kg/m <sup>3</sup>	295.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives

rho	1134.10	kg/m <sup>3</sup>	297.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1133.50	kg/m <sup>3</sup>	298.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1132.60	kg/m <sup>3</sup>	299.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1131.80	kg/m <sup>3</sup>	300.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1130.40	kg/m <sup>3</sup>	302.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1129.60	kg/m <sup>3</sup>	303.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1128.90	kg/m <sup>3</sup>	304.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives

rho	1127.50	kg/m <sup>3</sup>	306.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1125.90	kg/m <sup>3</sup>	308.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1124.70	kg/m <sup>3</sup>	310.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1123.50	kg/m <sup>3</sup>	312.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1122.60	kg/m <sup>3</sup>	313.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1121.20	kg/m <sup>3</sup>	315.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rho	1120.00	kg/m <sup>3</sup>	317.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives

rho1	1119.30	kg/m3	318.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
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## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.20	K	3.70	NIST Webbook

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C100550&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives

<https://www.doi.org/10.1016/j.fluid.2012.10.024>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

## 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>rho1:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tf:</b>	Normal melting (fusion) point

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