

Nicotinyl alcohol

Other names:	.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
Inchi:	InChI=1S/C6H7NO/c8-5-6-2-1-3-7-4-6/h1-4,8H,5H2
InchiKey:	MVQVNTPHUGQQHK-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	OCc1cccnc1
Mol. weight [g/mol]:	109.13
CAS:	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	1100.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1119.00		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 ³	291.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1137.50	kg/m ³	292.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1136.80	kg/m ³	293.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives
rhoI	1135.30	kg/m ³	295.15	A comparative study of the volumetric properties of aqueous solutions of pyridine and piperidine derivatives

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

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

McGowan Method:

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

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>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rho1:	Liquid Density
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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