

# Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-

## Other names:

(-)-3-(1-Methyl-2-pyrrolidyl)pyridine  
(-)-3-(N-Methylpyrrolidino)pyridine  
(-)-Nicotine  
(-)-«beta»-Pyridyl-«alpha»-N-methylpyrrolidine  
(-)-Â«betaÂ»-Pyridyl-Â«alphaÂ»-N-methylpyrrolidine  
(S)-(-)-Nicotine  
(S)-3-(1-Methyl-2-pyrrolidinyl)pyridine  
(S)-Nicotine  
1-Methyl-2-(3-pyridyl)pyrrolidine  
1-Methyl-2-(3-pyridyl)pyrrolidine  
3-(1-Methyl-2-pyrrolidinyl)pyridine  
3-(1-Methyl-2-pyrrolidinyl)pyridine  
3-(2-(N-methylpyrrolidinyl))pyridine  
3-(N-Methylpyrrolidino)pyridine  
Black Leaf  
Black Leaf 40  
Campbell's nico-soap  
Destruxol orchid spray  
Emo-Nik  
Flux MAAG  
Fumetobac  
Habitrol  
L-3-(1-Methyl-2-pyrrolidyl)pyridine  
L-Nicotine  
Mach-Nic  
NSC 5065  
Niagara P.A. dust  
Nic-Sal  
Nico-Dust  
Nico-Fume  
Nicocide  
Nicoderm  
Nicotin  
Nicotina  
Nicotine  
Nicotine alkaloid  
Nicotrol  
Nikotin  
Nikotyne  
Ortho N-4 and N-5 dusts

Ortho N-4 dust  
Ortho N-5 dust  
Pyridine, 3-(tetrahydro-1-methylpyrrol-2-yl), (S)-  
Pyrrolidine, 1-methyl-2-(3-pyridyl)-  
S-(-)-nicotine  
Tendust  
XL All Insecticide  
niconil

**Inchi:** InChI=1S/C10H14N2/c1-12-7-3-5-10(12)9-4-2-6-11-8-9/h2,4,6,8,10H,3,5,7H2,1H3/t10-/m  
**InchiKey:** SNICXCGAKADSCV-SNVBAGLBSA-N  
**Formula:** C10H14N2  
**SMILES:** CN1CCCC1c1cccnc1  
**Mol. weight [g/mol]:** 162.23  
**CAS:** 54-11-5

## Physical Properties

Property code	Value	Unit	Source
affp	963.40	kJ/mol	NIST Webbook
basg	932.60	kJ/mol	NIST Webbook
hvap	63.90 ± 2.10	kJ/mol	NIST Webbook
log10ws	0.79		Aqueous Solubility Prediction Method
logp	1.848		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
rinpol	1360.50		NIST Webbook
rinpol	1360.50		NIST Webbook
ripol	1863.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hvapt	63.90	kJ/mol	298.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hvapt	46.10	kJ/mol	448.00	NIST Webbook
pvap	8.21e-03	kPa	303.30	Thermodynamic properties of S-(-)-nicotine
pvap	3.51e-03	kPa	293.80	Thermodynamic properties of S-(-)-nicotine
pvap	5.52e-03	kPa	298.50	Thermodynamic properties of S-(-)-nicotine
pvap	2.40e-03	kPa	288.70	Thermodynamic properties of S-(-)-nicotine
pvap	0.01	kPa	308.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.01	kPa	308.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.02	kPa	313.10	Thermodynamic properties of S-(-)-nicotine
pvap	0.03	kPa	318.10	Thermodynamic properties of S-(-)-nicotine
pvap	0.04	kPa	323.00	Thermodynamic properties of S-(-)-nicotine
pvap	0.05	kPa	327.90	Thermodynamic properties of S-(-)-nicotine
pvap	0.07	kPa	333.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.08	kPa	335.70	Thermodynamic properties of S-(-)-nicotine
pvap	0.10	kPa	338.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.11	kPa	340.70	Thermodynamic properties of S-(-)-nicotine
pvap	0.14	kPa	343.10	Thermodynamic properties of S-(-)-nicotine

pvap	0.16	kPa	345.60	Thermodynamic properties of S-(-)-nicotine
pvap	0.21	kPa	348.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.22	kPa	350.60	Thermodynamic properties of S-(-)-nicotine
pvap	0.27	kPa	353.20	Thermodynamic properties of S-(-)-nicotine
pvap	500.02	kPa	609.30	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	0.51	kPa	363.20	Thermodynamic properties of S-(-)-nicotine
pvap	0.67	kPa	368.10	Thermodynamic properties of S-(-)-nicotine
pvap	0.86	kPa	373.10	Thermodynamic properties of S-(-)-nicotine
pvap	14.96	kPa	447.70	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	19.93	kPa	457.20	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	29.87	kPa	471.10	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	49.83	kPa	490.60	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry

pvap	79.61	kPa	510.10	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	99.84	kPa	520.40	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	247.84	kPa	566.40	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	397.81	kPa	594.80	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
pvap	0.37	kPa	358.10	Thermodynamic properties of S-(-)-nicotine
pvap	568.97	kPa	617.80	Vapor pressure data of nicotine, anabasine and cotinine using differential scanning calorimetry
rho1	1010.23	kg/m3	293.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures
rho1	985.96	kg/m3	323.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures
rho1	1002.10	kg/m3	303.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures

rho1	998.05	kg/m3	308.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures
rho1	994.01	kg/m3	313.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures
rho1	989.98	kg/m3	318.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures
rho1	1006.16	kg/m3	298.15	Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures

## Sources

Thermodynamic and spectroscopic interpretation of molecular interactions of nicotine + alcohol binary mixtures: High pressure phase behavior of binary (CO<sub>2</sub> + nicotine) and ternary (CO<sub>2</sub> + nicotine + toluene) mixtures: CO<sub>2</sub> liquid phase solubility in nicotine systems containing nicotine: Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids: Crippen Method:

<https://www.doi.org/10.1016/j.jct.2016.07.005>

KDB:

<https://www.doi.org/10.1016/j.fluid.2009.04.008>

Thermodynamic properties of S-(-)-nicotine: Liquid-liquid equilibria of imidazolium ionic liquids having bistriflamide or triflate anions with aromatic, non-polar and polar compounds: Liquid-liquid phase equilibria in nicotine (aqueous) solutions: McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2007.02.016>

<https://www.doi.org/10.1021/je2001446>

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

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1489>

<https://www.doi.org/10.1016/j.jct.2018.01.014>

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpy and Heat Capacity of Nicotine and Nicotinic Acid and Related Compounds: Scanning calorimetry:

<https://www.doi.org/10.1016/j.fluid.2012.10.007>

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

<https://www.doi.org/10.1016/j.fluid.2011.08.022>

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

<https://www.doi.org/10.1021/je900034d>

<https://www.doi.org/10.1016/j.tca.2014.08.033>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54115&Units=SI>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinp:</b>	Non-polar retention indices
<b>rip:</b>	Polar retention indices

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