

Niacin

Other names:

3-Carboxypyridine
3-Carboxypyridine
3-Pyridinecarboxylic acid
3-Pyridylcarboxylic acid
Acide nicotinique
Acidum nicotinicum
Akotin
Apelagrin
Bionic
Daskil
Davitamon PP
Diacin
Direktan
Efacin
Kyselina nikotinova
Linic
NAH
NICO
Naotin
Niac
Niacor
Niaspan
Nicacid
Nicamin
Nicangin
Nico-400
Nico-Span
Nicobid
Nicocap
Nicocidin
Nicocrisina
Nicodan
Nicodelmine
Nicodon
Nicolar
Niconacid
Niconat
Niconazid
Nicolor
Nicosan 3

Nicoside
Nicosyl
Nicotamin
Nicotene
Nicotil
Nicotine acid
Nicotinic acid
Nicotinipca
Nicotinsaure
Nicovasan
Nicovasen
Nicovel
Nicyl
Nipellen
Nyclin
P.P. factor
P.P. factor-pellagra preventive factor
PP Factor
Pellagra preventive factor
Pellagramin
Pellagrin
Pelonin
Peviton
Pyridine-3-carboxylic acid
Pyridine-carboxylique-3
Pyridine-«beta»-carboxylic acid
Pyridine-Â«betaÂ»-carboxylic acid
S115
SK-Niacin
Tega-Span
Tinic
Vitamin B3
Vitaplex N
Wampocap
anti-Pellagra vitamin
m-Pyridinecarboxylic acid
«beta»-Pyridinecarboxylic acid
Â«betaÂ»-Pyridinecarboxylic acid
Inchi: InChI=1S/C6H5NO2/c8-6(9)5-2-1-3-7-4-5/h1-4H,(H,8,9)
InchiKey: PVNIIMVLHYAWGP-UHFFFAOYSA-N
Formula: C6H5NO2
SMILES: O=C(O)c1cccnc1
Mol. weight [g/mol]: 123.11

Physical Properties

Property code	Value	Unit	Source
chs	-2730.67 ± 0.57	kJ/mol	NIST Webbook
chs	-2730.83 ± 0.48	kJ/mol	NIST Webbook
hf	-221.50 ± 1.50	kJ/mol	NIST Webbook
hfs	-344.90 ± 0.90	kJ/mol	NIST Webbook
hfs	-344.97 ± 0.67	kJ/mol	NIST Webbook
hfs	-344.81 ± 0.92	kJ/mol	NIST Webbook
hsub	123.90 ± 3.70	kJ/mol	NIST Webbook
hsub	105.20 ± 0.60	kJ/mol	NIST Webbook
hsub	123.40 ± 1.20	kJ/mol	NIST Webbook
hsub	123.40 ± 1.20	kJ/mol	NIST Webbook
ie	9.38	eV	NIST Webbook
log10ws	-0.71		Aqueous Solubility Prediction Method
logp	0.780		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
tf	510.48 ± 0.50	K	NIST Webbook
tf	510.26	K	Solubility of Nicotinic Acid and Nicotinamide in Carbon Dioxide at T = (313.15 to 373.15) K and p = (5 to 30) MPa: Experimental Data and Correlation
tf	510.06	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.70	kJ/mol	510.00	NIST Webbook
hfust	97.10	kJ/mol	509.30	NIST Webbook

hfust	27.57	kJ/mol	509.10	NIST Webbook
hfust	30.00	kJ/mol	510.00	NIST Webbook
hsubt	101.10 ± 0.60	kJ/mol	362.00	NIST Webbook
hsubt	89.30	kJ/mol	485.50	NIST Webbook
rhos	1460.00	kg/m3	250.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1454.00	kg/m3	275.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1444.00	kg/m3	300.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1465.00	kg/m3	225.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1430.00	kg/m3	350.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1422.00	kg/m3	375.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1413.00	kg/m3	400.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1406.00	kg/m3	425.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1471.00	kg/m3	200.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1477.00	kg/m3	175.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3
rhos	1481.00	kg/m3	150.00	Thermodynamic properties and low-temperature X-ray diffraction of vitamin B3

rhos

1436.00

kg/m³

325.00

Thermodynamic
properties and
low-temperature
X-ray diffraction
of vitamin B3

Sources

McGowan Method:

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

Volumetric and viscometric studies of
nicotinic acid in aqueous solutions of
sodium chloride at T = (298.15 to 308.15) K:

<https://www.doi.org/10.1016/j.jct.2016.03.010>

Source: Solubility Prediction Method

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

Solubility of Niacin in 3-Picoline +

<https://www.doi.org/10.1021/je034165+>

Water from (287.65 to 359.15) K:

Solvation behavior of some vitamins in
aqueous solutions of sodium chloride

<https://www.doi.org/10.1016/j.tca.2013.08.007>

Densities and viscosities of Niacin +

<https://www.doi.org/10.1021/je0496387>

3-Picoline + Water from (298.15 to 313.15) K:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

On the solubility of nicotinic acid and
isonicotinic acid in water and organic
solvents:

<https://www.doi.org/10.1016/j.jct.2013.01.024>

Volumetric and viscometric studies on

<https://www.doi.org/10.1016/j.tca.2012.10.017>

L-ascorbic acid, nicotinic acid,

niacin, riboflavin and folic acid:

<https://www.doi.org/10.1021/je100774p>

Conductance of a ternary solution of

<https://www.doi.org/10.1021/je0496995>

3-Picoline + Water Mixtures from

<https://www.doi.org/10.1021/je100697a>

Solubility of Nicotinic Acid and

Nicotinamide in Carbon Dioxide at T =

<https://www.doi.org/10.1016/j.jct.2014.02.024>

(298.15 to 313.15) K: A density and

viscosity study of nicotinic

<https://www.doi.org/10.1016/j.tca.2015.01.012>

acid and nicotinic acid in

carbon dioxide at different

temperatures and the

temperature for the maximum density of

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C59676&Units=SI>

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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