

Niacinamide

Other names: 3-(Aminocarbonyl)pyridine
3-Amidopyridine
3-Carbamoylpyridine
3-Pyridinecarboxylic acid amide
3-pyridinecarboxamide
Acid amide
Amid kyseliny nikotinove
Amide PP
Aminicotin
Amixicotyn
Amnicotin
Austrovit PP
Benicot
Delonin Amide
Dipegyl
Dipigyl
Endobion
Factor PP
Hansamid
Inovitan PP
NAM
Nandervit-N
Niacevit
Niamide
Niavit PP
Nicamide
Nicamina
Nicamindon
Nicasir
Nicobion
Nicoft
Nicogen
Nicomidol
Nicosan 2
Nicosylamide
Nicota
Nicotamide
Nicotilamide
Nicotililamido
Nicotine acid amide

Nicotinic amide
Nicotinsaureamid
Nicitol
Nicotylamide
Nicovel
Nicovit
Nicovitina
Nicovitol
Nicozymin
Nictoamide
Niko-tamin
Nikotinamid
Nikotinsaeureamid
Niocinamide
Niozymin
PP-Faktor
Papulex
Pelmin
Pelmine
Pelonin Amide
Pyridine, 3-carbamoyl-
Pyridine-3-carboxylic acid amide
Savacotyl
Vi-Nicotyl
Vi-noctyl
Vitamin B
Vitamin B3
Vitamin PP
Witamina PP
b-Pyridinecarboxamide
nicotinamide
nicotinic acid amide
«beta»-Pyridinecarboxamide

Inchi: InChI=1S/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)

InchiKey: DFPAKSUCGFBDDF-UHFFFAOYSA-N

Formula: C6H6N2O

SMILES: N=C(O)c1cccnc1

Mol. weight [g/mol]: 122.12

CAS: 98-92-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	0.965		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
tf	401.70	K	(Solid + liquid) phase diagram for (indomethacin + nicotinamide)- methanol or methanol/ethyl acetate mixture and solubility behavior of 1:1 (indomethacin + nicotinamide) co-crystal at T = (298.15 and 313.15) K
tf	404.15	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
tt	398.50	K	Solubility Determination of Nicotinamide and Its Application for the Cocrystallization with Benzoic Acid

Sources

Crippen Method:

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 of Nicotinamide Cocrystals in Ethanol and Ethanol/Water Mixtures at McGowan Method (298.15 and 313.15) K:

Solubility and Mass Transfer Coefficient Enhancement of Stearic Acid by Indomethacin in Supercritical (Solid + liquid) Phase Diagram for (indomethacin + nicotinamide)-Partial Molar Volumes and Viscosity Coefficients of Nicotinamide in 1:1 (indomethacin + nicotinamide) co-crystal and its application for the cocrystallization with Benzoic Acid: nicotinamide and Indomethacin co-crystal formation, Self-Interactions of Nicotinamide and its solvation and viscosity Coefficients of nicotinamide and its pressure-solubility enhancement in supercritical CO₂ and its application with supercritical CO₂ as an anti-solvent:

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

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

<https://www.doi.org/10.1021/je5011455>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C98920&Units=SI>

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

<https://www.doi.org/10.1021/je901041n>

<https://www.doi.org/10.1016/j.jct.2015.01.015>

<https://www.doi.org/10.1007/s10765-009-0567-5>

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

<https://www.doi.org/10.1021/acs.jced.8b00560>

<https://www.doi.org/10.1016/j.fluid.2013.11.024>

<https://www.doi.org/10.1021/je500447r>

<https://www.doi.org/10.1016/j.jct.2007.09.012>

<https://www.doi.org/10.1016/j.fluid.2014.03.029>

https://www.chemeo.com/doc/models/crippen_log10ws

Investigation on Molecular Interactions of Nicotinamide in Aqueous Citric Acid Solutions with Reference to Manifestation of Partial Molar Volume and Viscosity B-Coefficient

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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