

Isoniazid

Other names:

4-(Hydrazinocarbonyl)pyridine
4-Pyridinecarbonylhydrazine
4-Pyridinecarboxylic acid, hydrazide
4-Pyridylcarbonyl hydrazide
4-pyridinecarboxylic hydrazide
4-pyridylcarbonylhydrazide
5015 R.P.
Amidon
Andrazide
Antimicina
Antituberkulosum
Armacide
Armazid
Armazide
Atcotibine
Azuren
BP 5015
Bacillin
Cedin
Cemidon
Chemiazid
Chemidon
Cortinazine
Cotinazin
Cotinizin
Defonin
Dibutin
Diforin
Dinacrin
Ditubin
Ebidene
Eralon
Ertuban
Eutizon
Evalon
FSR 3
Fimalene
GINK
HIA
Hidranizil

Hidrasonil
Hidrulta
Hidrun
Hycozid
Hydrazid
Hyozyd
Hyzyd
IN-73
INAH
INH
Ido-tebin
Idrazil
Inizid
Iscotin
Isidrina
Ismazide
Isobicina
Isocid
Isocidene
Isocotin
Isohydrazide
Isolyn
Isonazid
Isonerit
Isonex
Isoniacid
Isoniazid SA
Isoniazide
Isonicazide
Isonicid
Isonico
Isonicotan
Isonicotil
Isonicotinhydrazid
Isonicotinic acid hydrazide
Isonicotinic hydrazide
Isonicotinohydrazide
Isonicotinoyl hydrazide
Isonicotinylhydrazide
Isonicotinylhydrazine
Isonide
Isonidrin
Isonikazid

Isonilex
Isonin
Isonindon
Isonirit
Isoniton
Isonizide
Isotebezid
Isozide
Isozyd
Laniazid
Mayambutol
Mybasan
NSC 9659
Neoteben
Neoxin
Neumandin
Nevin
Niadrin
Nicetal
Nicizina
Niconyl
Nicotibina
Nicotisan
Nicozide
Nidaton
Nidrazid
Nikozid
Niplen
Nitadon
Nydrazid
Nyscozid
Pelazid
Preparation 6424
Pycazide
Pyricidin
Pyridine-4-carbohydrazide
Pyrizidin
RU-EF-Tb
Raumanon
Retozide
Rimicid
Rimifon
Rimiphone

Rimitsid
Robisellin
Sauterazid
TB-Razide
TB-Vis
Tebecid
Teebaconin
Tekazin
Tibinide
Tibizide
Tisin
Tisiodrazida
Tizide
Tubazid
Tubazide
Tubeco
Tubicon
Tubilysin
Tubomel
Tyvid
Unicozyde
Vazadrine
Vederon
Zidafimia
Zinadon
Zonazide

[(4-Pyridinylcarbonyl)oxy]hydrazine

Inchi: InChI=1S/C6H7N3O/c7-9-6(10)5-1-3-8-4-2-5/h1-4H,7H2,(H,9,10)
InchiKey: QRXWMOHMRWLFY-UHFFFAOYSA-N
Formula: C6H7N3O
SMILES: NNC(=O)c1ccncc1
Mol. weight [g/mol]: 137.14
CAS: 54-85-3

Physical Properties

Property code	Value	Unit	Source
hfus	27.91	kJ/mol	A favourable solubility of isoniazid, an antitubercular antibiotic drug, in alternative solvents

hfus	31.10			Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol
log10ws	0.01			Aqueous Solubility Prediction Method
log10ws	9.00e-03			Estimated Solubility Method
logp	-0.315			Crippen Method
mcvol	103.150		ml/mol	McGowan Method
rinpol	1582.00			NIST Webbook
rinpol	1582.00			NIST Webbook
tf	445.84		K	Solubility Data as a Response for a Challenge for Formulation Chemists: Imidazolium-Based Ionic Liquids and Antitubercular Antibiotic Medicines
tf	444.47		K	Aqueous Solubility Prediction Method
tf	445.84		K	Ammonium ionic liquids as green solvents for drugs
tf	445.84		K	Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds
tf	445.84		K	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid
tt	446.04		K	Solubility and Data Correlation of Isoniazid in Different Pure and Binary Mixed Solvent Systems from 283.15 K to 323.15 K

Sources

Estimated Solubility Method:

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds

<https://www.doi.org/10.1016/j.fluid.2014.10.033>

Organic Solvents from (30) to (12) K: Volumetric, acoustic and viscometric studies of solute-solute and solute-solvent interactions

<https://www.doi.org/10.1021/je800156m>

Solute-solvent interactions in supercritical CO₂-D-glucose/sucrose solutions

<https://www.doi.org/10.1016/j.jct.2019.01.024>

Ammonium ionic liquids as green solvents for drugs: Ternary mutual diffusion of isoniazid in aqueous sodium chloride, sodium

<https://www.doi.org/10.1021/je900622h>

Binary Mutual Diffusion Coefficients of Isoniazid Aqueous Solutions at (298.15 and 310.15) K:

<https://www.doi.org/10.1016/j.fluid.2012.11.029>

<https://www.doi.org/10.1016/j.jct.2010.02.014>

<https://www.doi.org/10.1021/je900221m>

Solubility and Data Correlation of Isoniazid in Different Pure and Binary Solvents: A Response to the 2016 K Challenge for Formulation Chemists: A Data-Driven Approach to Solubility Prediction Method: An Alternative Solvents!

<https://www.doi.org/10.1021/acs.jced.8b00785>

Solvation thermodynamics of anti-tuberculosis Isoniazid in aqueous and non-aqueous media: A McGowan Method-based prediction method: NIST Webbook:

<https://www.doi.org/10.1021/acs.jced.6b00201>

Crippen Method:

<https://www.doi.org/10.1016/j.fluid.2012.01.022>

Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol:

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

<https://www.doi.org/10.1016/j.jct.2018.04.003>

<https://www.doi.org/10.1016/j.fluid.2015.03.053>

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54853&Units=SI>

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

<https://www.doi.org/10.1016/j.jct.2015.08.022>

Legend

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

tt: Triple Point Temperature

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