



Formula: C₁₀H₁₄N₂

MW: 162.23

CAS: 54-11-5

MDL: MFCD00071696

TNP: TNP00391

1-METHYL-2-(3-PYRIDYL)PYRROLIDINE; BLACK LEAF 40; (+/-)-NICOTINE; NICOTINE; (+)-nicotin; (+)-pyridin; (r,s)-nicotine; 3-(1-methyl-2-pyrrolidinyl)-pyridin



LogP: 3.33

LogS: -3.69

Acceptors: 0

Donors: 0

Rotation Bonds: 0

Chiral Centers: 1

N+O: 2

LIPINSKY: 4

Oil: LIQUID

Info: L-Nicotine 99+%

IUPAC: 3-((2S)-1-methylpyrrolidin-2-yl)pyridine

Smiles: C1N([C@@H](CC1)c1cnccc1)C

Specification: Nicotine Derivatives; Agonists/Ion Channels; Cholinergics; Ligand-Gated Ion Channels; Neurotransmitters; Nicotinic Acetylcholine Receptor Modulators (+/-)-NICOTINE
Chemical Properties:

density 1.02 g/mL at 25 C(lit.) Fp 101 C solubility ethanol: 50 mg/mL form liquid color yellow
CAS DataBase Reference 22083-74-5(CAS DataBase Reference) Safety Information Hazard
Codes T+,N Risk Statements 25-27-51/53 Safety Statements 36/37-45-61 RIDADR UN 1654
6.1/PG 2 WGK Germany 3 RTECS QS5257500 (+/-)-NICOTINE Usage And Synthesis
Chemical Properties:

Colourless Liquid Usage This is the unnatural isomer of Nicotine (+/-)-NICOTINE Raw
materials CALCIUM CARBONATE

Merck 13 Reference: Monograph Number: 0006551

Title: Nicotine

CAS Registry Number: 54-11-5

CAS Name: 3-[(2S)-1-Methyl-2-pyrrolidinyl]pyridine

Additional Names: 1-methyl-2-(3-pyridyl)pyrrolidine; b-pyridyl-a-N-methylpyrrolidine

Trademarks: Habitrol (Novartis); Nicabate (GlaxoSmithKline); Nicoderm CQ
(GlaxoSmithKline); Nicolan (Elan); Nicopatch (Fabre); Nicotinell (Novartis); NiQuitin CQ
(GlaxoSmithKline); Tabazur (Th