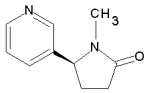

Formula: C10H12N2O

MW: 176.22

CAS: 486-56-6

MDL: MFCD00219442

TNP: TNP00100

1-METHYL-5-[3-PYRIDYL]-2-PYRROLIDINONE; L-COTININE; (-)-COTININE; COTININE; S-(-)-COTININE; (S)-(-)-1-METHYL-5-(3-PYRIDIYL)-2-PYRROLIDINONE; [S]-1-METHYL-5-[3-PYRIDYL]-2-PYRROLIDINONE; S(-)-1-METHYL-5-(3-PYRIDYL)-2-PYRROLIDONE

LogP: 7.44

LogS: -6.03

Acceptors: 1

Donors: 0

Rotation Bonds: 0

Chiral Centers: 1

N+O: 3

LIPINSKY: 3

Oil: OIL

IUPAC: (5S)-1-methyl-5-(3-pyridyl)pyrrolidin-2-one

Smiles: N1([C@@H](CCC1=O)c1cnccc1)C

Specification: Various Metabolites and Impurities; Metabolites; Nicotine Derivatives
(-)-COTININE Chemical Properties:

mp 40-42 C(lit.) bp 250 C150 mm Hg(lit.) Fp >230 F storage temp. 2-8C Merck 14,2553 BRN 83099 Stability:Stable. Incompatible with strong oxidizing agents. May be heat sensitive - store cold. Safety Information Hazard Codes Xn,Xi Risk Statements 22-36/37/38 Safety Statements 7-16-36/37-45-36-26 RIDADR UN 1230 3/PG 2 WGK Germany 3 RTECS GN1925500 F 10
(-)-COTININE Usage And Synthesis Chemical Properties:

Colourless to Light Brown Solid UsageA major metabolite of nicotine in humans Biological ActivityMajor metabolite of nicotine. Shown to activate a subpopulation of a 3/ a 6