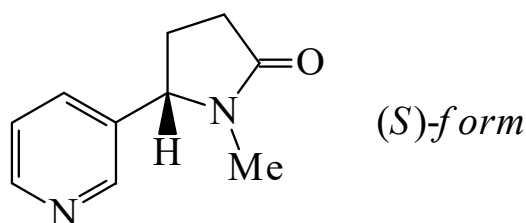




>>Entry Name: Cotinine, INN

Synonym(s): 1-Methyl-5-(3-pyridinyl)-2-pyrrolidinone, 9CI



CAS Registry Number: 75202-09-4

Molecular Formula: C₁₀H₁₂N₂O

Molecular Weight: 176.218

Accurate Mass: 176.094963

Percentage Composition: C 68.16%; H 6.86%; N 15.90%; O 9.08%

Physical Description: Viscous oil

Development Status: Never marketed

Boiling Point: Bp₆ 210-211°

Calculated Log P Data: Log P -0.47 (uncertain value) (calc)

>>Variant: (S)-form

CAS Registry Number: 486-56-6

Molecular Formula: C₁₀H₁₂N₂O

Molecular Weight: 176.218

Accurate Mass: 176.094963

Percentage Composition: C 68.16%; H 6.86%; N 15.90%; O 9.08%

Biological Source: Alkaloid from leaf tobacco (*Nicotiana tabacum*), also detected in *Duboisia hopwoodii* (Solanaceae)

Biological Use/Importance: Antidepressant. Nicotine metabolite, used as a biomarker for exposure to cigarette smoke. Shows behavioural effects in animals

Melting Point: Mp 40-43°

Boiling Point: Bp 210-211° 6

Other Data: V. hygroscopic. Prob. artifact of autoxidn. of nicotine

Hazard & Toxicity: LD₅₀ (mus, orl) 1604 mg/kg. LD₅₀ (mus, ipr) 930 mg/kg

Aldrich: 28471-8

Fluka: 27699

Sigma: C5923

>>Derivative: Fumarate (2:1)

Synonym(s): Cotinine fumarate, USAN. Scotine

CAS Registry Number: 5695-98-7

>>Derivative: Picrate

Melting Point: Mp 102-103°

>>Variant: (±)-form

CAS Registry Number: 15569-85-4

Molecular Formula: C₁₀H₁₂N₂O

Molecular Weight: 176.218

Accurate Mass: 176.094963

Percentage Composition: C 68.16%; H 6.86%; N 15.90%; O 9.08%

Source/Synthesis: Synthetic

Physical Description: Yellow oil

Boiling Point: Bp 210-211°

References: