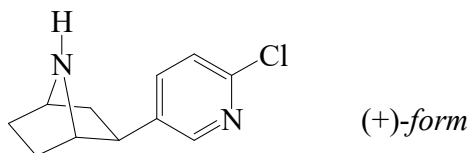




>>Entry Name: Epibatidine

Synonym(s): 2-(6-Chloro-3-pyridinyl)-7-azabicyclo[2.2.1]heptane, 9Cl



Type of Compound Code(s): XA0650

Molecular Formula: C₁₁H₁₃ClN₂

Molecular Weight: 208.69

Accurate Mass: 208.076725

Percentage Composition: C 63.31%; H 6.28%; Cl 16.99%; N 13.42%

General Statement: Unique new class of alkaloids

Calculated Log P Data: Log P 1.02 (calc)

UV: [neutral] λ_{max} 217 (ε); 270 (sh) (ε); 274 (ε 5300) (MeOH) (Derep) [acid] λ_{max} (solvent not reported) (Derep)

>>Variant: (+)-form

CAS Registry Number: 140111-52-0

Type of Compound Code(s): VX1040 XA3140

Molecular Formula: C₁₁H₁₃ClN₂

Molecular Weight: 208.69

Accurate Mass: 208.076725

Percentage Composition: C 63.31%; H 6.28%; Cl 16.99%; N 13.42%

Biological Source: Alkaloid from the skin extracts of the Ecuadoran poison frog *Epipedobates tricolor*

Biological Use/Importance: Neuronal nicotinic acetylcholine receptor agonist (most potent known to date). Also active at neuromuscular nicotinic receptors. Potent non-opioid analgesic (potency reported to be 200-500 times greater than that of morphine)

Melting Point: Mp 56-57°

Optical Rotation: [α]_D²³+5 (c, 0.35 in CHCl₃)

Other Data: Data refer to synthetic material

>>Derivative: Hydrochloride

Melting Point: Mp 150 dec.°

Optical Rotation: [α]_D²⁴+34.7 (c, 0.36 in MeOH)

>>Variant: (–)-form

CAS Registry Number: 152378-30-8

Molecular Formula: C₁₁H₁₃ClN₂

Molecular Weight: 208.69

Accurate Mass: 208.076725

Percentage Composition: C 63.31%; H 6.28%; Cl 16.99%; N 13.42%

Physical Description: Needles

Melting Point: Mp 56-57°. Mp 64°

Optical Rotation: [α]_D²³–5 (c, 0.35 in CHCl₃)

Other Data: Similar pharmacol. profile to (+)-form

>>Derivative: Hydrochloride

Melting Point: Mp 130 dec.°

Optical Rotation: [α]_D²⁴–33.7 (c, 0.16 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 148152-66-3

Molecular Formula: C₁₁H₁₃ClN₂

Molecular Weight: 208.69

Accurate Mass: 208.076725

Percentage Composition: C 63.31%; H 6.28%; Cl 16.99%; N 13.42%

Source/Synthesis: Synthetic

Melting Point: Mp 50-51°