



>>>Derivative: *N*-Oxide (axial O)

Synonym(s): Hyoscyamine *N*-oxide 2

CAS Registry Number: 56362-74-4

Molecular Formula: C₁₇H₂₃NO₄

Molecular Weight: 305.373

Accurate Mass: 305.162709

Percentage Composition: C 66.86%; H 7.59%; N 4.59%; O 20.96%

Biological Source: Alkaloid from *Atropa*, *Datura*, *Hyoscyamus*, *Scopolia* and *Mandragora* spp.

Melting Point: Mp 175-180 dec.° (as hydrochloride)

>>>Derivative: *N*-De-Me

Synonym(s): Norhyoscyamine

CAS Registry Number: 537-29-1

Molecular Formula: C₁₆H₂₁NO₃

Molecular Weight: 275.347

Accurate Mass: 275.152144

Percentage Composition: C 69.79%; H 7.69%; N 5.09%; O 17.43%

Biological Source: Alkaloid from aerial parts of *Datura meteloides*. The major alkaloid of some strains of *Duboisia myoporoides* (Solanaceae)

>>>Variant: (±)-form

Synonym(s): Atropine, BAN, INN, USAN

CAS Registry Number: 51-55-8

Molecular Formula: C₁₇H₂₃NO₃

Molecular Weight: 289.374

Accurate Mass: 289.167794

Percentage Composition: C 70.56%; H 8.01%; N 4.84%; O 16.59%

Biological Source: Alkaloid from *Atropa belladonna*, *Datura stramonium* and other Solanaceae

Use/Importance: Mydriatic, antispasmodic and cycloplegic agent. Smooth muscle relaxant. Used in preanaesthetic medication to prevent reflex brachycardia and bronchospasm and to decrease gland secretions. Reduces rigidity in parkinsonism. Antidote to poisoning with parasympathomimetic agents, e.g. nerve gases, organophosphorus insecticides. Cause of deliberate and accidental poisoning of humans and livestock. Nontoxic to some spp., e.g. rabbits. Reference material used in elemental microanalysis

Melting Point: Mp 116-117°

Solubility: BERDY SOL: Sol. MeOH, CHCl₃, acids; fairly sol. Et₂O, C₆H₆; poorly sol. H₂O, hexane

pKa Value: pK_a 10.2 (25°)

Calculated Log P Data: Log P 1.32 (calc)

Other Data: In many cases, Atropine may be an artifact of the extraction procedure

Hazard & Toxicity: Adverse human effects by ingestion, and other routes of administration, incl. dryness of the mouth, difficulty swallowing and thirst. Adverse ocular effects. Can cause death. Variable human lethal dose, but 100 mg can be fatal. LD₅₀ (rat, orl) 500 mg/kg. Exp. reprod. and teratogenic effects

Fluka: 11320

Rare Chemicals Library: S44566-5

Sigma: A0132

>>>Derivative: Hydrobromide

CAS Registry Number: 6415-90-3

Melting Point: Mp 163-164°

>>>Derivative: Sulfate (2:1)

Synonym(s): Atropine sulfate, JAN, USAN. Atropisol

CAS Registry Number: 55-48-1

Physical Description: Cryst.

Melting Point: Mp 190-194°

Other Data: Component of Antrocol, Colonaïd, Donnagel, Kinesed, Lomotil and Hydrapred

Hazard & Toxicity: Human systemic effects. LD₅₀ (rat, orl) 600 mg/kg. Exp. reprod. and teratogenic effects

>>>Derivative: Picrate

Melting Point: Mp 175-176°