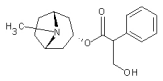

Formula: C17H23NO3

MW: 289.37

CAS: 51-55-8

MDL: MFCD00022622

TNP: TNP00272

ATROPINE; (+/-)-HYOSCYAMINE; HYOSCYAMINE; DL-HYOSCYAMINE; TIMTEC-BB SBB005985; (+,-)-Tropyl tropate; (+,-)-tropyltropate; 1alphaH,5alphaH-Tropan-3alpha-ol (

LogP: 3.07

LogS: -4.23

Acceptors: 3

Donors: 1

Rotation Bonds: 4

Chiral Centers: 3

N+O: 4

LIPINSKY: 4

IUPAC: (1S,5R)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl 3-hydroxy-2-phenylpropanoate

Smiles: N1([C@@H]2C[C@@H](OC(C(c3ccccc3)CO)=O)C[C@H]1CC2)C

THERAPEUTIC CATEGORY: Antiholinergic; mydriatic.

VET THERAPEUTIC CATEGORY:Anticholinergic; mydriatic; antispasmodic

SOURCE: Parasympatholyc alkaloid isolated from Atropa beladonna L.,and other Solanaceae.

Biochem-Physiol Action: Competitive nonselective antagonist at central and peripheral muscarinic acetylcholine receptors.

Merck Reference:

Monograph Number: 0000879
Title: Atropine
CAS Registry Number: 51-55-8
CAS Name: a-(Hydroxymethyl)benzeneacetic acid (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester
Additional Names: 1aH,5aH-tropan-3a-ol (±)-tropate (ester); dl-hyoscyamine; tropic acid ester with tropine; dl-tropyl tropate; tropine tropate
Molecular Formula: C17H23NO3
Molecular Weight: 289.37.
Percent Composition: C 70.56%, H 8.01%, N 4.84%, O 16.59%
Literature References: Parasympatholytic alkaloid isolated from Atropa belladonna L., Datura stramonium L., and other Solanaceae. Extraction procedure: Chemnitius, J. Prakt. Chem. 116, 276 (1927). During extraction, partial racemization of the l-hyoscyamine takes place which is completed by treatment with dil alkali on heating in chloroform soln: Schneider, Arch. Pharm. 284, 306 (1951). Structure and synthesis: Ladenburg, Ann. 217, 75 (1883); Willstätter, Ber. 31, 1537 (1898); idem., Ann. 326, 23 (1903); Schwenker et al., Ber. 99, 2407 (1966). Prepn of the sulfate: DE 247455 (1912 to Hoffmann-La Roche), Frdl. 11, 1022. Use as antidote to cholinesterase inhibitors: R. V. Brown, Br. J. Pharmacol. 15, 170 (1960). Effect on cardiac arrhythmias: P. Schweitzer, H. Mark, Am. Heart J. 100, 119, 255 (1980). Pharmacokinetics and pharmacodynamics: P. H. Hinderling et al., J. Pharm. Sci. 74, 703, 711 (1985). Toxicity: R. L. Cahen, K. Tvede, J. Pharmacol. Exp. Ther. 105, 166 (1952); Goldenthal, Toxicol. Appl. Pharmacol. 18, 185 (1971). Review of clinical use in anesthesia: L. E. Shutt, J. B. Bowes, Anaesthesia 34, 476-490 (1979). Comprehensive description: A. A. Al-Badr, F. J. Muhtadi, Anal. Profiles Drug Subs. 14, 325-389 (1985). Review of clinical toxicology: J. D. Truwit, Crit. Care Clin. 7, 639-657 (1991).
Properties: Long, orthorhombic prisms from acetone, mp 114-116°. Sublimes in high vacuum at 93-110°. pK 4.35; pH of 0.0015 molar soln 10.0. Absorption spectra: Dobbie, Fox, J. Chem. Soc. 103, 1194 (1913); Fischer, Arch. Exp. Pathol. Pharmakol. 170, 623 (1933). One gram dissolves in 455 ml water, 90 ml water at 80°, 2 ml alc, 1.2 ml alc at 60°, 27 ml glycerol, 25 ml ether, 1 ml chloroform; also sol in benzene, dil acids. LD50 orally in rats: 750 mg/kg (Cahen, Tvede).
Melting point: mp 114-116°
pKa: pK 4.35; pH of 0.0015 molar soln 10.0
Toxicity data: LD50 orally in rats: 750 mg/kg (Cahen, Tvede)

Derivative Type: Methylbromide
CAS Registry Number: 2870-71-5
Additional Names: Methylatropine bromide
Trademarks: Tropin (Takeda)
Molecular Formula: C17H23NO3.CH3Br
Molecular Weight: 384.31.
Percent Composition: C 56.25%, H 6.82%, N 3.64%, O 12.49%, Br 20.79%

Properties: Crystals, mp 222-223°. Sol in 1 part water; slightly sol in alc. Almost insol in chloroform, ether.
Melting point: mp 222-223°

Derivative Type: Methylnitrate
CAS Registry Number: 52-88-0
Additional Names: Methylatropine nitrate
Trademarks: Eumydrin (SKB)
Molecular Formula: C17H23NO3.CH3NO3
Molecular Weight: 366.41.
Percent Composition: C 59.00%, H 7.15%, N 7.65%, O 26.20%
Properties: Crystals, mp 163°. Freely sol in water or alc, very slightly in chloroform, ether.
Melting point: mp 163°

Derivative Type: Sulfate monohydrate
CAS Registry Number: 5908-99-6; 55-48-1 (anhydrous)
Trademarks: Atropisol (Novartis); Atropt (Sigma)
Molecular Formula: (C17H23NO3)2.H2SO4.H2O
Molecular Weight: 694.83.
Percent Composition: C 58.77%, H 7.25%, N 4.03%, O 25.33%, S 4.61%
Properties: Granules or powder, mp 190-194°. Almost inactive optically. Very bitter. pH ~5.4. One gram dissolves in 0.4 ml water; 5 ml cold, 2.5 ml boil. alc; in 2.5 ml glycerol, 420 ml chloroform, 3000 ml ether. Bitterness threshold 1:10,000. Incompatible with alkalies, tannin, salts of mercury or gold, vegetable decoctions or infusions, borax, bromides, iodides, benzoates. LD50 orally in rats: 622 mg/kg (Goldenthal).
Melting point: mp 190-194°
Toxicity data: LD50 orally in rats: 622 mg/kg (Goldenthal)

Derivative Type: N-Oxide
CAS Registry Number: 4438-22-6
Additional Names: Atropine aminoxide; aminoxytropine tropate; genatropine
Molecular Formula: C17H23NO4
Molecular Weight: 305.37.
Percent Composition: C 66.86%, H 7.59%, N 4.59%, O 20.96%
Literature References: Prepn: Polonovski, Polonovski, Bull. Soc. Chim. Fr. 39, 1147 (1926).
Properties: Crystalline powder, mp 127-128°, dec 135°. Very hygroscopic. Soluble in alc, chloroform. Practically insol in ether.
Melting point: mp 127-128°

CAUTION: Causes blurred vision, suppressed salivation, vasodilation, hyperpyrexia, excitement, agitation, and delirium. See: Clinical Toxicology of Commercial Products, R. E. Gosselin et al., Eds. (Williams & Wilkins, Baltimore, 5th Ed., 1984) Section III, pp 47-50.
Therap-Cat: Mydriatic; antispasmodic. In preanesthetic medication.
Therap-Cat-Vet: Mydriatic; antispasmodic. Antidote to organophosphorus insecticides.