



Formula: C₂₁H₂₂N₂O₂

MW: 334.42

CAS: 57-24-9

MDL: MFCD03225437

TNP: TNP00295

(-)-STRYCHNINE; STRYCHNINE; Strychnidin-10-one; STRYCHNINE ALKALOID; Vauquiline; L-STRYCHNINE;
2,4a,5,5a,7,8,15,15a,15b,15c-decahydro-4,6-methano-6h,14h-indolo[3,2,1-ij]oxep;
4,6-Methano-6H,14H-indolo[3,2,1-ij]oxepino[2,3,4-de]pyrrolo[2,3-h]quinoline, strychnidin



LogP: 2.03

LogS: -3.46

Acceptors: 2

Donors: 0

Rotation Bonds: 0

Chiral Centers: 6

N+O: 4

LIPINSKY: 4

Info: in seeds of *Strychnos nuxvomica* L. and beans of *S. Ignatica*. USE in poison baits for rodents

IUPAC:

(11S,18S,22S,1R,20R,21R)-12-oxa-8,17-diazaheptacyclo[15.5.2.0.0.0.0.0]tetracos-2,4,6,14-te

traen-9-one

Smiles:

C1N2[C@@H]3([C]4([C@H]5(N(C(=O)C[C@H]6([C@@H]5([C@H](C3)(C1=CCO6))))c1c4cccc1))CC2)

Specification: Alkaloids; Biochemistry; for Resolution of Acids; Indole Alkaloids; Optical Resolution; Synthetic Organic Chemistry **STRYCHNINE** Chemical Properties:

mp 284-286 C(lit.) storage temp. Poison room solubility chloroform: clear to hazy Merck 8855 Stability:Stable. Incompatible with strong oxidizing agents. CAS DataBase Reference57-24-9(CAS DataBase Reference) Safety Information Hazard Codes T+,N Risk Statements 27/28-50/53 Safety Statements 36/37-45-60-61 RIDADR UN 1692 6.1/PG 1 WGK Germany 3 RTECS WL2275000 HazardClass 6.1(a) PackingGroup I **STRYCHNINE** Usage And Synthesis Chemical Properties:

white crystals or powder General DescriptionColorless, transparent crystals or white crystalline powder. Has no odor. Used for destroying rodents and predatory animals and for trapping fur-bearing animals. Reactivity Profile**STRYCHNINE** is an alkaloid derivative. **STRYCHNINE** is a base and forms water soluble salts with acids. Avoid alkalis, alkali carbonates and bicarbonates, benzoates, dichromates, bromides, iodides, tannic and picric acids, salicylates, borax, gold chloride and other alkaloid precipitants, piperazine, potassium-mercuric iodide. Protect from light. [EPA, 1998]. **STRYCHNINE** is incompatible with the following: Strong oxidizers . Health HazardSuper toxic; probable oral lethal dose in humans is less than 5 mg/kg, a taste (less than 7 drops) for a 70 kg (150 lb.) person. It causes violent generalized convulsions. Death results from respiratory arrest as the respiratory muscles are in sustained spasm. The lowest lethal oral dose reported for humans is 30 mg/kg. Fire HazardWhen heated, emits highly toxic fumes. Fire may produce irritating or poisonous gases. Runoff from fire control or dilution water may cause pollution. Protect from light. **STRYCHNINE**

Merck 13 Reference: Monograph Number: 0008937

Title: Strychnine

CAS Registry Number: 57-24-9

CAS Name: Strychnidin-10-one

Molecular Formula: C₂₁H₂₂N₂O₂

Molecular Weight: 334.41.

Percent Composition: C 75.42%, H 6.63%, N 8.38%, O 9.57%

Literature References: Occurs most abundantly in seeds of *Strychnos nux-vomica* L., Loganiaceae and beans of *S. ignatti*, Berg. One of the first alkaloids isolated in pure form.

Isoln: Pelletier, Caventou, Ann. Chim. Phys. 8, 323 (1818); *ibid.* 10, 142 (1819). Extraction procedure: C. Srinivasulu et al., Res. Ind. 23, 224 (1978). Structure elucidation: L. H. Briggs et al., J. Chem. Soc. 1946, 903; H. T. Openshaw, R. Robinson, Nature 157, 438 (1946); R. B. Woodward et al., J. Am. Chem. Soc. 69, 2250 (1947). Total synthesis: R. B. Woodward et al., *ibid.* 76, 4749 (1954); *eidem*, Tetrahedron 19, 247 (1963). Abs config: A. F. Peerdeman, Acta Crystallogr. 9, 824 (1956); K. Nagarajan et al., Helv. Chim. Acta 46, 1212 (1963). Stereoselective total synthesis: S. D. Knight et al., J. Am. Chem. Soc. 115, 9293 (1993). ¹H- and ¹³C-NMR analysis: E. Wenkert et al., J. Org. Chem. 43, 1099 (1978). Pharmacology and pharmacokinetics: S. Weiss, R. A. Hatcher, J. Pharmacol. Exp. Ther. 19, 419 (1921). Acute toxicity: I. Setnikar, M. J. Magistretti, Arzneim.-Forsch. 14, 996 (1964). HPLC determ in urine and tissues: T. Egloff et al., J. Clin. Chem. Clin. Biochem. 20, 203 (1982). Review: J. B. Hendrickson in The Alkaloids vol. VI, R. H. F. Manske, Ed. (Academic Press, New York, 1960) pp 179-195; G. F. Smith, *ibid.* vol. VIII (1965) pp 591-671. Comprehensive description: F. J. Muhtadi, M. S. Hifnawy, Anal. Profiles Drug Subs. 15, 563-646 (1986). Brief review of synthesis: U. Beifuss, Angew. Chem. Int. Ed. 33, 1144-1149 (1994).

Properties: Brilliant, colorless cubes from chloroform-ether, mp 275-285. d₁₈ 1.359. [α]_D18 -104.3 (c = 0.254 in alc); [α]_D25 -139 (c = 0.4 in chloroform). pK_a (25) 8.26: A. J. Everett et al., J. Chem. Soc. 1957, 1120. uv max (95% ethanol): 255, 280, 290 nm (E1%1 cm 377, 130, 101): A. I. Biggs, J. Pharm. Pharmacol. 13, 547 (1952). One gram dissolves in 182 ml ethanol, 6.5 ml chloroform, 150 ml benzene, 250 ml methanol, 83 ml pyridine; very slightly soluble in ether, water. Bitter taste in soln contg 1 part in 700,000 of water. LD₅₀ i.v. (slow infusion) in rats: 0.96 mg/kg (Setnikar, Magistretti).

pK_a: pK_a (25) 8.26: A. J. Everett et al., J. Chem. Soc. 1957, 1120

Optical Rotation: [α]_D18 -104.3 (c = 0.254 in alc); [α]_D25 -139 (c = 0.4 in chloroform)

Absorption maximum: uv max (95% ethanol): 255, 280, 290 nm (E1%1 cm 377, 130, 101): A. I. Biggs, J. Pharm. Pharmacol. 13, 547 (1952)

Density: d₁₈ 1.359

Toxicity data: LD₅₀ i.v. (slow infusion) in rats: 0.96 mg/kg (Setnikar, Magistretti)

Derivative Type: Acetate

Molecular Formula: C₂₃H₂₆N₂O₄

Molecular Weight: 394.46.

Percent Composition: C 70.03%, H 6.64%, N 7.10%, O 16.22%

Properties: Crystals, sol in 20 parts water, sol in alcohol.

Derivative Type: Gluconate pentahydrate

Molecular Formula: C₂₇H₃₄N₂O₉·5H₂O

Molecular Weight: 620.64.

Percent Composition: C 52.25%, H 7.15%, N 4.51%, O 36.09%

Properties: Crystals, darken above 80, sol in 2 parts water, ~40 parts alcohol; the aq soln is neutral.

Derivative Type: Glycerophosphate hexahydrate

Molecular Formula: C₄₅H₅₃N₄O₁₀P·6H₂O

Molecular Weight: 948.99.

Percent Composition: C 56.95%, H 6.90%, N 5.90%, O 26.98%, P 3.26%

Properties: One gram dissolves in ~350 ml water, ~310 ml alcohol. Slightly sol in chloroform; very slightly in ether.

Derivative Type: Hydrochloride dihydrate

Molecular Formula: C₂₁H₂₃ClN₂O₂·2H₂O

Molecular Weight: 406.90.

Percent Composition: C 61.99%, H 6.69%, Cl 8.71%, N 6.88%, O 15.73%

Properties: Efflorescent, trimetric prisms. One gram dissolves in ~40 ml water, ~80 ml alc. Insol in ether. pH of 0.01M soln 5.4.

Derivative Type: Nitrate see separate entry

Derivative Type: Phosphate see separate entry

Derivative Type: Salicylate

Molecular Formula: C₂₈H₂₈N₂O₅

Molecular Weight: 472.53.

Percent Composition: C 71.17%, H 5.97%, N 5.93%, O 16.93%

Properties: Leaflets, sol in ~30 parts water; sparingly sol in alcohol.

Derivative Type: Sulfate see separate entry

CAUTION: Extremely poisonous, see: G. D. Osweiler, Curr. Vet. Ther. 6, 115 (1977). Potential symptoms of overexposure to strychnine are stiff neck and facial muscles; restlessness, apprehension and increased acuity of perception; increased reflex excitability; cyanosis; tetanic convulsions with opisthotonos. See NIOSH Pocket Guide to Chemical Hazards (DHHS/NIOSH 97-140, 1997) p 286.

Use: Chiefly in poison baits for rodents.

Therap-Cat-Vet: Has been used as a tonic and central stimulant.