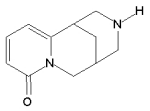

Formula: C11H14N2O

MW: 190.25

CAS: 485-35-8

TNP NUMBER: TNP00030

MDL NUMBER: MFCD00075715

IUPAC: 7,11-diazatricyclo[7.3.1.0]trideca-2,4-dien-6-one

Smiles: C1NCC2c3n(c(ccc3)=O)CC1C2

in seeds Laburnum Anagiroides and other Leguminosae

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 2

LogP: 0.86

LogS: -3.09

LIPINSKI: 4

Monograph Number: 0002818

Title: Cytisine

CAS Registry Number: 485-35-8

CAS Name: (1R)-1,2,3,4,5,6-Hexahydro-1,5-methano-8H-pyrido-[1,2-a][1,5]diazocin-8-one

Additional Names: baptitoxine; sophorine; ulexine

Trademarks: Cytiton (USSR)

Molecular Formula: C11H14N2O

Molecular Weight: 190.24.

Percent Composition: C 69.45%, H 7.42%, N 14.73%, O 8.41%

Literature References: Toxic principle in seed of Laburnum anagyroides Medik. and other Leguminosae. Extraction: Ing, J. Chem. Soc. 1931, 2200; Spath, Galinovsky, Ber. 65, 1526 (1932); 66, 1338 (1933); Lecoq, Bull. Soc. Chim. Fr. 10, 153 (1943). Structure: Ing, J. Chem. Soc. 1932, 2778. Synthesis: Bohlmann et al., Angew. Chem. 67, 708 (1955); Van Tamelen, Baran, J. Am. Chem. Soc. 77, 4944 (1955). Absolute configuration: Okuda et al., Chem. Ind. (London) 1961, 1751. Pharmacological properties: R. B. Barlow, L. J. McLeod, Br. J. Pharmacol. 35, 161 (1969).

Properties: Orthorhombic prisms from acetone, mp 152-153. Sublimes. bp2 218. [a]D17 -120. pK1 6.11; pK2 13.08. Sol in 1.3 parts water, 13 parts acetone, 1.3 parts methanol, 3.5 parts alcohol, 30 parts benzene, 10 parts ethyl acetate, 2.0 parts chloroform. Practically insol in petr ether. LD50 in mice (mg/kg): 1.73 i.v.; 9.4 i.p.; 101 orally (Barlow, McLeod).

Melting point: mp 152-153

Boiling point: bp2 218

pKa: pK1 6.11; pK2 13.08

Optical Rotation: [a]D17 -120

Toxicity data: LD50 in mice (mg/kg): 1.73 i.v.; 9.4 i.p.; 101 orally (Barlow, McLeod)

Derivative Type: Hydrochloride

Molecular Formula: C11H14N2O.HCl

Molecular Weight: 226.70.

Percent Composition: C 58.28%, H 6.67%, N 12.36%, O 7.06%, Cl 15.64%

Properties: Deliquescent crystals, sol in water and alcohol. pH of 0.1 molar aq soln 4.3.

Derivative Type: Nitrate monohydrate

Molecular Formula: C11H14N2O.HNO3.H2O

Molecular Weight: 271.27.

Percent Composition: C 48.70%, H 6.32%, N 15.49%, O 29.49%

Properties: Needles or leaflets, [a]D -81.5. Sol in water, slightly sol in alcohol. Practically insol in ether.

Optical Rotation: [a]D -81.5

Synonyms:
SOPHORINE;1,2,3,4,5,6-Hexahydro-1,5-methano-8H-pyrido[1,2-a][1,5]diazocin-8-one;1,2,3,4,5,6-Hexahydro-1,5-methano-pyrido[1,2-a][1,5]diazocin;1,5-Methano-8H-pyrido(1,2-a)(1,5)diazocin-8-one, 1,2,3,4,5,6-hexahydro-;1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R)-;1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R-cis)-;2-a)(1,5)diazocin-8-one,1,2,3,4,5,6-hexahydro-5-methano-8h-pyrido(1;5)diazocin-8-one,1,2,3,4,5,6-hexahydro-5-methano-8h-pyrido((1r)-2-a)(1

CAS:485-35-8

MF:C11H14N2O

MW:190.24

EINECS:207-616-0

Product Categories:Heterocyclic Compounds;Neurochemicals;Nicotine Derivatives CYTISINE

Chemical Properties: mp 154-156 C(lit.) bp 218 C2 mm Hg(lit.) storage temp. Store at RT form powder color light yellow Merck 13,2818 NIST Chemistry ReferenceCytisine(485-35-8) EPA

Substance Registry System1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R,5S)-(485-35-8) T Risk Statements 25-36/37/38 Safety Statements 26-28-36/37-45 RIDADR UN 2811 6.1/PG 3 WGK Germany 3 RTECS HA4025000 HazardClass 6.1(b) PackingGroup III Hazardous Substances Data485-35-8(Hazardous Substances Data) CYTISINE

Usage And Synthesis:

Chemical Properties: Off-White to Tan Crystalline Solid UsageToxic priniciple in seed of Laburnum anagyroides and other Leguminosae. A neuronal nicotinic acetylcholine agonist Biological ActivityA potent, selective agonist at neuronal nicotinic receptors. Acts as a partial agonist at B 2-containing nicotinic receptors. CYTISINE