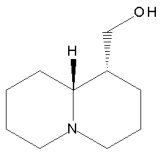

Formula: C10H19NO

MW: 169.27

CAS: 487-70-4

TNP NUMBER: TNP00032

MDL NUMBER: MFCD01083034

IUPAC: ((1R,2R)-6-azabicyclo[4.4.0]dec-2-yl)methan-1-ol

Smiles: C1CN2CCCC[C@@H]2([C@@H](C1)CO)

REFERENCE: Mirzaev S. Farmakol Toksikol. 41:52-5 (1978).

SOURCE: An alkaloid isolate from Anabisis aphylla

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 1

N+O: 2

Chiral Centers: 2

LogP: 1.79

LogS: -3.29

LIPINSKI: 4

Monograph Number: 0005630

Title: Lupinine

CAS Registry Number: 486-70-4

CAS Name: [1R-trans]-Octahydro-2H-quinolizine-1-methanol

Additional Names: l-lupinine; (-)-lupinine

Molecular Formula: C10H19NO

Molecular Weight: 169.26.

Percent Composition: C 70.96%, H 11.31%, N 8.28%, O 9.45%

Literature References: Naturally occurring l-form isolated from seeds and herb of Lupinus luteus L. and other L. species, Leguminosae also found in Anabasis aphylla L., Chenopodiaceae. Extraction procedure: J. F. Couch, J. Am. Chem. Soc. 56, 2434 (1934). Structure and synthesis: R. W. Willstatter, E. Fourneau, Ber. 35, 1910 (1902); P. Karrer et al., Helv. Chim. Acta 11, 1062 (1928); K. Winterfeld, F. W. Holschneider, Ber. 64B, 137, 692 (1931); K. Winterfeld, ibid. 692. Synthesis of racemic lupinine: F. W. Holschneider, K. Winterfeld, Arch. Pharm. 277, 192 (1939); G. C. Gerrans et al., Tetrahedron Lett. 1975, 4171; T. Iwashita et al., J. Org. Chem. 47, 230 (1982). Synthesis of racemic lupinine and epi-lupinine: G. R. Clemo et al., J. Chem. Soc. 1937, 965; H. Takahata et al., Chem. Pharm. Bull. 34, 4523 (1986); of l-epi-lupinine: M. L. Bremmer, S. M. Weinreb, Tetrahedron Lett. 24, 261 (1983). Absolute configuration of (-)-form: R. C. Cookson, Chem. Ind. (London) 1953, 339. Crystal structure: A. Koziol et al., Acta Crystallogr. B34, 3491 (1978). Biosynthesis: Soucek, Schutte, Angew. Chem. 74, 901 (1962); W. M. Golebiewski, I. D. Spenser, J. Am. Chem. Soc. 106, 1441 (1984).

Properties: Stout, orthorhombic prisms from acetone, mp 68.5-69.2. bp4 160-164; bp755 269-270. [a]D26 -25.9 (c = 3 in water); [a]D28 -21 (c = 9.5 in alcohol). Sol in water, alcohol, chloroform, ether. It is a strong base.

Melting point: mp 68.5-69.2

Boiling point: bp4 160-164; bp755 269-270

Optical Rotation: [a]D26 -25.9 (c = 3 in water); [a]D28 -21 (c = 9.5 in alcohol)

Derivative Type: l-Form hydrochloride

Molecular Formula: C10H20ClNO

Molecular Weight: 205.72.

Percent Composition: C 58.38%, H 9.80%, Cl 17.23%, N 6.81%, O 7.78%

Properties: Orthorhombic prisms, mp 208-213. [a]D -14.

Melting point: mp 208-213

Optical Rotation: [a]D -14

Derivative Type: dl-Form

Properties: Crystals from acetone, mp 58.5-59.5.

Melting point: mp 58.5-59.5

Synonyms:
OCTAHYDRO-1H-QUINOLIZIN-1-METHANOL;LUPININ;(-)-LUPININE;LUPININE;(1R-TRANS)-OCTAHYDRO-2H-QUINOLIZINE-1-METHANOL;(1R,9AR)-1-(OCTAHYDRO-QUINOLIZIN-1-YL)-METHANOL;(1R,9AR)-OCTAHYDRO-2H-QUINOLIZIN-1-YLMETHANOL;2H-Quinolizine-1-methanol, octahydro-, (1R-trans)-

CAS:486-70-4

MF:C10H19NO

MW:169.26

EINECS:207-638-0

Product Categories:Alkaloids (-)-LUPININE

Chemical Properties: mp 62-65C bp 160-164C 4mm Fp 160-164C/4mm Merck 14,5609 BRN 80447

CAS DataBase Reference: 486-70-4(

CAS DataBase Reference:) NIST Chemistry Reference2H-quinolizine-1-methanol, octahydro-, (1r-trans)-(486-70-4) Xi Risk Statements 20/21/22 Safety Statements 22-36/37 RIDADR 1544 RTECS OK5802000 Hazard Note Irritant HazardClass 6.1 PackingGroup III (-)-LUPININE

Usage And Synthesis: (-)-LUPININE