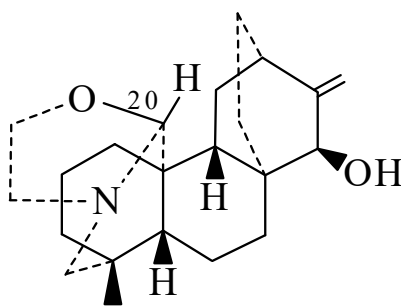




>>Entry Name: Atisine, 9CI

Synonym(s): Anthorine



Absolute
configuration

CAS Registry Number: 466-43-3

Molecular Formula: $C_{22}H_{33}NO_2$

Molecular Weight: 343.508

Accurate Mass: 343.251129

Percentage Composition: C 76.92%; H 9.68%; N 4.08%; O 9.32%

General Statement: Exists as a mixt. of C-20 epimers in soln.

Biological Source: Alkaloid from *Aconitum heterophyllum*, *Aconitum gigas*, *Aconitum anthara* and *Aconitum heterophylloides* (Ranunculaceae)

Physical Description: Resin

Optical Rotation: $[\alpha]_D -21$ (c, 2.4 in EtOH). $[\alpha]_D -30.7$ (EtOH)

pKa Value: pK_a 12.8 (50% MeOH)

Other Data: Undergoes a ready isomerisation of the oxazolidine ring to Isoatisine [HGP61-C](#) on treatment with methanolic alkali or even by boiling MeOH

>>Derivative: Hydrochloride

Synonym(s): Atisinium chloride. Guan-fu base H

CAS Registry Number: 4758-99-0

Melting Point: Mp 311-312 (303°) dec.°

Optical Rotation: $[\alpha]_D^{25} +28$ (c, 1.10 in H_2O)

Other Data: Exists as a quaternary iminium salt rather than a protonated (^+NH) salt

References:

- Lawson, A. *et al.*, *J.C.S.*, 1937, 1640, (*isol*)
Jacobs, W.A. *et al.*, *J. Biol. Chem.*, 1942, **143**, 589, (*isol*)
Jacobs, W.A., *J.O.C.*, 1951, **16**, 1593, (*struct*)
Edwards, O.E. *et al.*, *Can. J. Chem.*, 1954, **32**, 465; 1955, **33**, 448, (*isol, uv, ir, struct*)
Wiesner, K. *et al.*, *Chem. Ind. (London)*, 1954, 132, (*struct*)
Pelletier, S.W. *et al.*, *J.A.C.S.*, 1954, **76**, 4496, (*struct*)
Nagata, W. *et al.*, *J.A.C.S.*, 1963, **85**, 2342, (*synth*)
Dvornik, D. *et al.*, *Can. J. Chem.*, 1964, **42**, 137, (*struct*)
Masamune, S., *J.A.C.S.*, 1964, **86**, 291, (*synth*)
Nagata, W. *et al.*, *J.A.C.S.*, 1967, **89**, 1483, (*synth*)
Pelletier, S.W. *et al.*, *Phytochemistry*, 1968, **7**, 625, (*isol, isom*)
Pelletier, S.W. *et al.*, *Tetrahedron*, 1968, **24**, 2019, (*pmr*)
Pradhan, S.K. *et al.*, *Chem. Comm.*, 1970, 644, (*struct*)
Scott, A.I. *et al.*, *Tetrahedron*, 1971, **27**, 4787, (*cd*)
Sakai, S. *et al.*, *Heterocycles*, 1977, **8**, 207, (*occur*)
Pelletier, S.W. *et al.*, *J.A.C.S.*, 1977, **99**, 284; 1978, **100**, 7976, (*cmr, cryst struct, abs config*)
Mody, N.V. *et al.*, *Tetrahedron*, 1978, **34**, 2421, (*cmr*)
Pelletier, S.W. *et al.*, *Tet. Lett.*, 1981, **22**, 313, (*occur*)
Shishido, K. *et al.*, *Chem. Comm.*, 1987, 1360, (*synth*)
Ihara, M. *et al.*, *J.A.C.S.*, 1990, **112**, 1164, (*synth*)
Banerjee, A.K., *Bull. Soc. Chim. Belg.*, 1994, **103**, 67, (*rev, synth*)