



Formula: C₂₀H₂₆N₂O₂

MW: 326.44

CAS: 4360-12-7

MDL: MFCD03225454

TNP: TNP00250

AJMALAN-17,21-DIOL,(17R,21)-; AJMALINE; 21-diol,(17r,21-alpha)-ajmalan-1;
5H-6,10:11,12a-Dimethanoindolo[3,2-b]quinolizine, ajmalan-17,21-diol deriv.;
Ajmalan-17,20-diol; Ajmalan-17,21-diol; Ajmalan-17,21-diol, (17R,21alpha)-; Ajmalin



LogP: 5.45

LogS: -5.91

Acceptors: 2

Donors: 2

Rotation Bonds: 0

Chiral Centers: 9

N+O: 4

LIPINSKY: 4

IUPAC:

(10S,13S,16S,1R,9R,14R,18R)-13-ethyl-8-methyl-8,15-diazahexacyclo[14.2.1.0.0.0.0]nonadeca-2,4,6-triene-14,18-diol

Smiles:

O[C@H]1[C@@]23[C@H]([C@H]4(N5[C@H](C1C(C4)[C@@H]([C@H]5O)CC)(C3)))(N(c1c2c

ccc1)C)

Specification: Alkaloids AJMALINE Chemical Properties:

mp 189C storage temp. 2-8C Merck 13,194 Safety Information Hazard Codes Xn Risk Statements 25-20/21/22 Safety Statements 13-45-36 RIDADR 1544 RTECS AX8050000 HazardClass 6.1(b) PackingGroup III AJMALINE Usage And Synthesis UsageAn antiarrhythmic agent isolated from Rauwolfia serpentina. AJMALINE

Merck 13 Reference: Monograph Number: 0000194

Title: Ajmaline

CAS Registry Number: 4360-12-7

CAS Name: Ajmalan-17,21-diol

Additional Names: rauwolfine

Trademarks: Aritmina (Altana); Gilurytmal (Solvay); Ritmos (Sanofi Synthelabo); Tachmalin (AWD)

Molecular Formula: C₂₀H₂₆N₂O₂

Molecular Weight: 326.43.

Percent Composition: C 73.59%, H 8.03%, N 8.58%, O 9.80%

Literature References: From roots of Rauwolfia serpentina (L.) Benth. (*Ophioxylon serpentinum* L.), Apocynaceae. Isolation: S. Siddiqui, R. H. Siddiqui, J. Indian Chem. Soc. 8, 667 (1931); 9, 539 (1932); 12, 37 (1935); L. van Itallie, A. J. Steenhauer, Arch. Pharm. 270, 313 (1932). Structure: A. Chatterjee, S. Bose, J. Indian Chem. Soc. 31, 17 (1954); F. A. L. Anet et al., J. Chem. Soc. 1954, 1242. Stereochemistry: M. F. Bartlett et al., J. Am. Chem. Soc. 84, 622 (1962). Synthesis: S. Masamune et al., *ibid.* 89, 2506 (1967); E. E. Van Tamelen, L. K. Oliver, *ibid.* 92, 2136 (1970); K. Mashimo, Y. Sato, Chem. Pharm. Bull. 18, 353 (1970). Physico-chemical properties: A. Petter, *Arzneim.-Forsch.* 24, 874 (1974). Antiarrhythmic activity: A. Petter, K. Engelmann, *ibid.* 876. Reviews: R. Robinson in *Festschrift Arthur Stoll* (Birkh