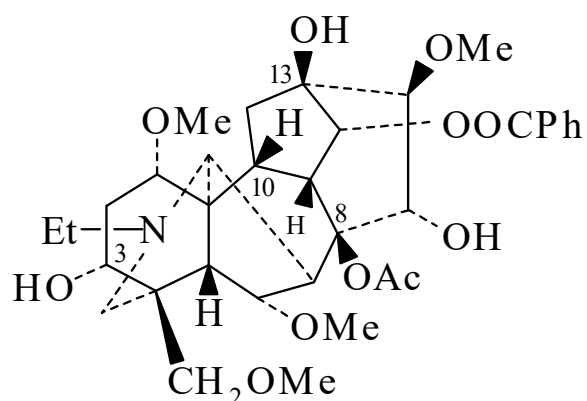




>>Entry Name: Aconitine



Absolute
configuration

CAS Registry Number: 302-27-2

Molecular Formula: $C_{34}H_{47}NO_{11}$

Molecular Weight: 645.745

Accurate Mass: 645.314914

Percentage Composition: C 63.24%; H 7.34%; N 2.17%; O 27.25%

Biological Source: Alkaloid from *Aconitum napellus*, *Aconitum fauriei*, *Aconitum grossedentatum*, *Aconitum hakusanense*, *Aconitum mokchangense*, *Aconitum zuccarini*, *Aconitum bullatifolium* var. *homotrichum*, *Aconitum carmichaeli*, *Aconitum karakolicum* and many others (Ranunculaceae)

Biological Use/Importance: Toxic agent implicated in poisoning by *Aconitum* spp., esp. *Aconitum chasmanthum* in India, exp. arrhythmia effects. Gastric anaesthetic. Homeopathic remedy against neuralgia and febrile diseases

Physical Description: Cryst.

Melting Point: Mp 204°

Optical Rotation: $[\alpha]_D +19$ (CHCl₃)

Solubility: V. spar. sol. H₂O

pKa Value: pK_a 8.35 (15°)

Other Data: Hydrol. to 4-Methylaconitane-1,3,6,8,13,14,15,16,18-nonol [CHG13-A](#)

Hazard & Toxicity: Very toxic if swallowed or by skin absorption. Human systemic effects by ingestion. LD₅₀ (mus, orl) 1 mg/kg, LD₅₀ (mus, ivn) 0.175 mg/kg, exp. lethal doses by subcutaneous route reported ; BERDY HAZD : LD₅₀ (mus, ivn) .166 mg/kg , LD₅₀ (mus, ipr) .328 mg/kg , LD₅₀ (mus, orl) 1 mg/kg

Aldrich: 28496-3

Fluka: 1570

Sigma: A8001

>>Derivative: Hydrochloride

Melting Point: Mp 170-172 dec.°

Optical Rotation: $[\alpha]_D -31$ (H₂O)

>>Derivative: O³-Ac

Synonym(s): Flaconitine. 3-Acetylaconitine

CAS Registry Number: 77181-26-1

Molecular Formula: $C_{36}H_{49}NO_{12}$

Molecular Weight: 687.783

Accurate Mass: 687.325479

Percentage Composition: C 62.87%; H 7.18%; N 2.04%; O 27.91%

Biological Source: Alkaloid from the roots of *Aconitum flavum* and *Aconitum pendulum* (Ranunculaceae)

Melting Point: Mp 196-197°

Optical Rotation: $[\alpha]_D^{24} +18.6$ (c, 1 in CHCl₃)

References:

Przybylska, M. *et al.*, *Can. J. Chem.*, 1959, **37**, 1116; 1843, (*struct*)

Bachelor, F.W. *et al.*, *Tet. Lett.*, 1960, **No. 10**, 1, (*struct*)

Birnbaum, K.B. *et al.*, *Tet. Lett.*, 1971, 867, (*config, struct*)

Chang, X. *et al.*, *Yaoxue Xuebao*, 1981, **16**, 474; *CA*, **97**, 3590f, (*Flaconitine*)

Wang, H. *et al.*, *Heterocycles*, 1985, **23**, 803, (*Flaconitine, cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, ADH750