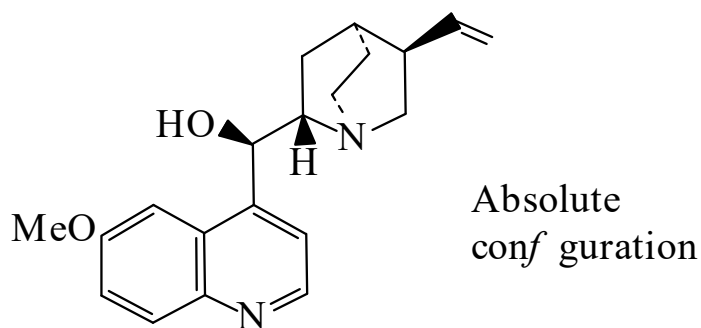




>>Entry Name: Quinine, BAN

Synonym(s): 6'-Methoxycinchonan-9-ol, 9Cl



CAS Registry Number: 130-95-0

Related CAS Registry Numbers(s): 6119-47-7 6119-70-6

Molecular Formula: $C_{20}H_{24}N_2O_2$

Molecular Weight: 324.422

Accurate Mass: 324.183778

Percentage Composition: C 74.05%; H 7.46%; N 8.63%; O 9.86%

Biological Source: Alkaloid from *Cinchona officinalis* and most other *Cinchona* spp., also in *Remijia pedunculata*. Occurs mainly in the bark (cinchona bark) but has also been isol. from trunkwood (Rubiaceae)

Use/Importance: Used as 1% aq. soln. (as sulfate) for photometric detn. of Bi, W, As(V), P(V). Resolving agent for organic acids, used in asymmetric syntheses.

Biological Use/Importance: Potassium channel blocker. Traditional antimalarial drug esp. important in treating *Plasmodium falciparum* which is resistant to other antimalarial drugs. Activity is stereochemistry-independent, i.e. racemates and stereoisomers show similar activity. Illicit abortifacient in large doses. Stimulant for horses, has been used in horse doping. Weak cardiac depressant, antipyretic and antifibrillatory agent

Physical Description: Cryst. with v. bitter taste

Melting Point: Mp 177° (anhyd.)

Optical Rotation: $[\alpha]_D -158$ (−145) (EtOH). $[\alpha]_D^{15} -158.7$ (Et₂O)

Solubility: Sol. H₂O, EtOH, C₆H₆, CHCl₃

pKa Value: pK_{a1} 8.34; pK_{a2} 4.21 (20°)

Calculated Log P Data: Log P 2.93 (calc)

Other Data: Forms a dihydrate and a trihydrate, Mp 57°(efflorescent). Triboluminescent. Blue fluor. in soln.

Hazard & Toxicity: Adverse effects from therapeutic or larger doses of quinine or its salts are collectively known as cinchonism. Irritant to mucous membranes. Human and exp. teratogenic effects. LD₅₀ (mus, ipr) 115 mg/kg

Aldrich: 14590-4

Fluka: 22620

>>Derivative: Hydrochloride

Synonym(s): Quinine hydrochloride, JAN. FEMA 1996

CAS Registry Number: 130-89-2

Extra CAS Registry Numbers(s): 7549-43-1

Physical Description: Needles + 2H₂O, dehydrating at 100°

Melting Point: Mp 158-160° (anhyd.)

Optical Rotation: $[\alpha]_D^{15} -145.5$ (EtOH)

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 60-93-5

Extra CAS Registry Numbers(s): 7549-43-1

Physical Description: Needles

Melting Point: Mp 180-185°

Optical Rotation: $[\alpha]_D^{18} -233$ (H₂O)

Hazard & Toxicity: LD₅₀ (rat, orl) 1393 mg/kg

Rare Chemicals Library: S45810-4

>>Derivative: Hydrobromide

CAS Registry Number: 549-49-5

Physical Description: Hygroscopic needles + H₂O

Melting Point: Mp 200° (softens from 152°)