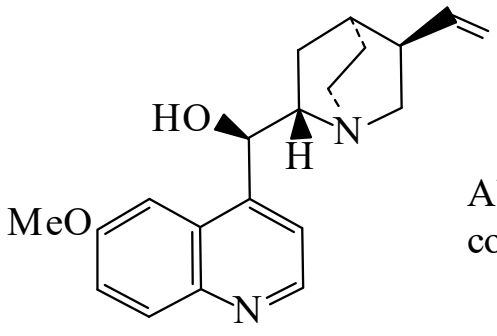
>>**Entry Name: Quinine,** BAN
Synonym(s): 6'-Methoxycinchonan-9-ol, 9CI



Absolute
conf guration

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 (Et_2O)
Solubility: Sol. H_2O, EtOH, C_6H_6, $CHCl_3$
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. LD_{50} (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 + $2H_2O$, 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 (H_2O)
Hazard & Toxicity: LD_{50} (rat, orl) 1393 mg/kg

Rare Chemicals Library: S45810-4

>>**Derivative:** Hydrobromide

CAS Registry Number: 549-49-5
Physical Description: Hygroscopic needles + H_2O
Melting Point: Mp 200° (softens from 152°)