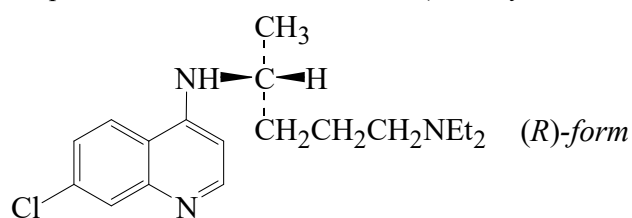




>>Entry Name: Chloroquine, BAN, INN

Synonym(s): N^4 -(7-Chloro-4-quinolinyl)- N^1,N^1 -diethyl-1,4-pentanediamine, 9Cl. 7-Chloro-4-(4-diethylamino-1-methylbutylamino)quinoline



CAS Registry Number: 54-05-7

Molecular Formula: $C_{18}H_{26}ClN_3$

Molecular Weight: 319.876

Accurate Mass: 319.181524

Percentage Composition: C 67.59%; H 8.19%; Cl 11.08%; N 13.14%

Use/Importance: Antimalarial, antiamoebic drug

Other Data: Component of Aablaquine

Hazard & Toxicity: Human reprod. and teratogenic effects. Common adverse effects incl. headaches, gastrointestinal disturbances, and skin eruptions, but high doses are cardiotoxic and cause severe visual effects. LD₅₀ (rat, orl) 330 mg/kg. Lethal human dose approx. 30 mg/kg

>>Variant: (R)-form

CAS Registry Number: 58175-87-4

Molecular Formula: $C_{18}H_{26}ClN_3$

Molecular Weight: 319.876

Accurate Mass: 319.181524

Percentage Composition: C 67.59%; H 8.19%; Cl 11.08%; N 13.14%

Physical Description: Cryst. (hexane)

Melting Point: Mp 65-67°

Optical Rotation: $[\alpha]_D^{20} -108.2$ (c, 1 in EtOH) (-86.2)

>>Variant: (S)-form

CAS Registry Number: 58175-86-3

Molecular Formula: $C_{18}H_{26}ClN_3$

Molecular Weight: 319.876

Accurate Mass: 319.181524

Percentage Composition: C 67.59%; H 8.19%; Cl 11.08%; N 13.14%

Melting Point: Mp 68-69°

Optical Rotation: $[\alpha]_D^{22} +108.2$ (c, 1 in EtOH)

Calculated Log P Data: Log P 4.92 (calc)

>>Derivative: Phosphate (1:2)

CAS Registry Number: 69698-55-1

Melting Point: Mp 202°

Optical Rotation: $[\alpha]_D^{22} +86.9$ (c, 2.1 in H₂O)

>>Variant: (±)-form

CAS Registry Number: 56598-66-4

Molecular Formula: $C_{18}H_{26}ClN_3$

Molecular Weight: 319.876

Accurate Mass: 319.181524

Percentage Composition: C 67.59%; H 8.19%; Cl 11.08%; N 13.14%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 87-88°

Boiling Point: Bp_{0.2} 212-214°

Calculated Log P Data: Log P 4.92 (calc)