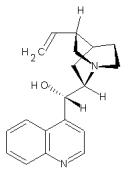

Formula: C19H22N2O

MW: 294.4

Salt: HCl, H2O

CAS: 118-10-5

TNP NUMBER: TNP00124

MDL NUMBER: MFCD00180253

IUPAC: ((5R)-5-vinylquinuclidin-2-yl)(1S)-4-quinolylmethan-1-ol

Smiles: c1(ccnc2c1cccc2)[C@@H]([C@H]1(CC2CC[N@@]1C[C@@H]2(C=C)))O

Occurs in most varieties of Cinchona bark, espesially in bark of Cinchona Micrantha R.

THERAPEUTIC CATEGORY: Antimalarial

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 3

N+O: 3

Chiral Centers: 4

LogP: 3.56

LogS: -4.53

LIPINSKI: 4

Synonyms:
D-CINCHONINE;(+)-CINCHONINE;CINCHONINE;CINCHONAN-9-OL,(9S)-;(+)-cinconine;(8r,9s)-cinchonine;(9s)-cinchonan-9-o;(9S)-Cinchonan-9-ol

CAS:118-10-5

MF:C19H22N2O

MW:294.39

EINECS:204-234-6

Product Categories:Miscellaneous Natural Products;chiral;Alkaloids;Biochemistry;for Resolution of Acids;Optical Resolution;Quinoline Alkaloids;Quinolinecarboxylic Acids, etc.;Quinolines;Synthetic Organic Chemistry;Asymmetric Synthesis;Chiral Resolution Reagents;Chiral Resolving ReagentsChiral Catalysts, Ligands, and Reagents;Cinchona Alkaloids;Privileged Ligands and Complexes Cinchonine

Chemical Properties: mp 260-263 C alpha 224 (c=0.5, alcohol) refractive index 223 (C=0.5, EtOH) Water Solubility Insoluble Sensitive Light Sensitive Merck 14,2287 BRN 89689 Stability:Stable, but may be light sensitive. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 118-10-5(

CAS DataBase Reference:) NIST Chemistry ReferenceCinchonine(118-10-5) EPA Substance Registry SystemCinchonan-9-ol, (9S)-(118-10-5) Xn Risk Statements 20/22-20/21/22 Safety Statements 26-36-36/37 RIDADR 1544 WGK Germany 3 RTECS GD3500000 F 8-34 HazardClass 6.1(b) PackingGroup III Cinchonine

Usage And Synthesis:

Chemical Properties: white to light yellow crystal powde Cinchonine