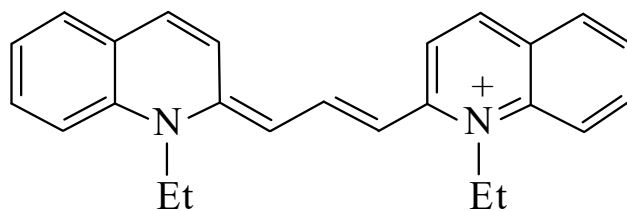




>>Entry Name: Pinacyanol

Synonym(s): 1-Ethyl-2-[3-(1-ethyl-2(1*H*)-quinolinylidene)propenyl]quinolinium(1+), 9Cl



Related CAS Registry Numbers(s): 2670-67-9

Molecular Formula: C₂₅H₂₅N₂⁽⁺⁾

Molecular Weight: 353.486

Accurate Mass: 353.201773

Percentage Composition: C 84.95%; H 7.13%; N 7.92%

>>Derivative: Chloride

Synonym(s): Quinaldine blue, INN, USAN. Pinacyanol chloride. Vernitest. NSC 56808

CAS Registry Number: 2768-90-3

Molecular Formula: C₂₅H₂₅ClN₂

Molecular Weight: 388.939

Accurate Mass: 388.170625

Percentage Composition: C 77.20%; H 6.48%; Cl 9.12%; N 7.20%

Use/Importance: Obstetric diagnostic aid. Non-intercalating dye, used as a biological stain

Physical Description: Blue-green prisms or needles (EtOH)

Melting Point: Mp 263° (dec.)

Other Data: Aq. soln. violet-red, alc. soln. blue

Aldrich: 20171-5

Sigma: P0392

>>Derivative: Bromide

CAS Registry Number: 2670-67-9

Molecular Formula: C₂₅H₂₅BrN₂

Molecular Weight: 433.39

Accurate Mass: 432.140109

Percentage Composition: C 69.29%; H 5.81%; Br 18.44%; N 6.46%

Melting Point: Mp 286 dec.°

Aldrich: 28198-0

Sigma: P9283

>>Derivative: Iodide

CAS Registry Number: 605-91-4

Molecular Formula: C₂₅H₂₅IN₂

Molecular Weight: 480.39

Accurate Mass: 480.106246

Percentage Composition: C 62.51%; H 5.25%; I 26.42%; N 5.83%

Melting Point: Mp 287-288°

Hazard & Toxicity: LD₅₀ (rat, ipr) 16 mg/kg

Aldrich: 16651-0

Fluka: 80560

Sigma: P5162

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