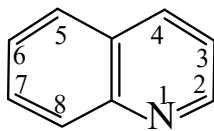




>>Entry Name: Quinoline

ENTRY UNDER REVIEW

Synonym(s): 1-Benzazine. 1-Azanaphthalene. FEMA 3470



CAS Registry Number: 91-22-5

Related CAS Registry Numbers(s): 1701-63-9 5436-28-2 26323-01-3 27926-80-3

Molecular Formula: C₉H₇N

Molecular Weight: 129.161

Accurate Mass: 129.057849

Percentage Composition: C 83.69%; H 5.46%; N 10.84%

Source/Synthesis: Occurs in coal tar and in ``stupp" fat. A fairly major constit. of cigarette smoke

Biological Source: Alkaloid from various plant spp. incl. *Mentha* spp., *Peganum harmala* and *Rubus laciniata*.

Use/Importance: Solv. for decarboxylations. Dehydrohalogenation reagent. Used for photometric detn. of Mo ($\lambda_{\max}$ 470 nm, ϵ 18000), gravimetric detn. of P(V); as a synergistic agent in extraction of Co

Biological Use/Importance: Antimalarial agent

Physical Description: Liq.

Melting Point: Fp -15.6°

Boiling Point: Bp 238.05°. Bp₁₇ 114°

Solubility: Mod. sol. H₂O

Density: d₄²⁰ 1.093

pKa Value: pK_a 4.9 (20°)

Refractive Index: n_D²⁰ 1.6268

Other Data: Hygroscopic, steam-volatile

Hazard & Toxicity: Fl. p. 99°, autoignition temp. 480°. Often violent synth. (Skraup reaction). Skin and severe eye irritant. Contact with liquid can damage eyes. LD₅₀ (rat, orl) 331 mg/kg. LD₅₀ (rbt, skn) 540 mg/kg. Reported to be mutagenic and carcinogenic

Aldrich: W34700-0

Fluka: 22660

>>Derivative: Hydrochloride

CAS Registry Number: 530-64-3

Physical Description: Deliquescent prisms + ½ H₂O

Melting Point: Mp 94°. Mp 134.5° (anhyd.)

>>Derivative: Sulfate (2:1)

CAS Registry Number: 54957-90-3

Physical Description: Cryst. (EtOH or AcOH)

Melting Point: Mp 163.5-164.5°

>>Derivative: Picrate

CAS Registry Number: 14876-03-0

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 207-208°

>>Derivative: N-Oxide

CAS Registry Number: 1613-37-2

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

Physical Description: Needles + 2H₂O

Melting Point: Mp 62°