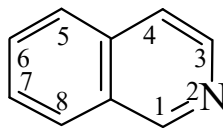




>>Entry Name: Isoquinoline, 9Cl, 8Cl

ENTRY UNDER REVIEW

Synonym(s): 2-Benzazine. Benzopyridine. 2-Azanaphthalene. FEMA 2978



CAS Registry Number: 119-65-3

Molecular Formula: C₉H₇N

Molecular Weight: 129.161

Accurate Mass: 129.057849

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

Biological Source: Isol. from the upper parts of *Spigelia anthelmia* (Spigeliaceae)

Use/Importance: Used for photometric detn. of Ni ($\lambda_{\max}$ 410 nm, ϵ 7900)

Physical Description: Hygroscopic cryst. or oil

Melting Point: Mp 25.5-26°

Boiling Point: Bp 242°. Bp₄₀ 142°

Solubility: Sol. EtOH, Et₂O, Me₂CO, C₆H₆

Density: d₄²⁰ 1.1

pKa Value: pK_a 5.4 (25°)

Hazard & Toxicity: Fl. p. >107°. Severe eye and skin irritant. LD₅₀ (rat, orl) 360 mg/kg. LD₅₀ (rbt, skn) 590 mg/kg

Aldrich: W29780-1

Fluka: 58750

Sigma: I2009

>>Derivative: Hydrochloride

CAS Registry Number: 21364-46-5

Physical Description: Needles (2-propanol/MeOH)

Melting Point: Mp 187-189°

>>Derivative: N-Me

Synonym(s): 1-Methylisoquinolinium(1+)

Molecular Formula: C₁₀H₁₀N⁽⁺⁾

Molecular Weight: 144.196

Accurate Mass: 144.081324

Percentage Composition: C 83.30%; H 6.99%; N 9.71%

Physical Description: Cryst. + 1H₂O (H₂O) (as iodide)

Melting Point: Mp 159° (iodide)

>>Derivative: N-Et

Synonym(s): N-Ethylisoquinolinium(1+)

Molecular Formula: C₁₁H₁₂N⁽⁺⁾

Molecular Weight: 158.223

Accurate Mass: 158.096974

Percentage Composition: C 83.50%; H 7.64%; N 8.85%

Physical Description: Yellow leaflets (EtOH)

Melting Point: Mp 148°

>>Derivative: Picrate

CAS Registry Number: 1567-46-0

Melting Point: Mp 226°

>>Derivative: N-Oxide