



>>Entry Name: 3-Aminoquinoline

Synonym(s): 3-Quinolinamine, 9Cl. β -Aminoquinoline

CAS Registry Number: 580-17-6

Molecular Formula: $C_9H_8N_2$

Molecular Weight: 144.176

Accurate Mass: 144.068748

Percentage Composition: C 74.98%; H 5.59%; N 19.43%

Physical Description: Cryst. (toluene, H_2O or EtOH aq.)

Melting Point: Mp 84°. Mp 94°

pKa Value: pK_a 4.91 (20°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 150 mg/kg

Aldrich: 23228-9

Fluka: 7338

Sigma: A5178

>>Derivative: Picrate

Melting Point: Mp 210 dec.°

>>Derivative: 3-N-Ac

CAS Registry Number: 5417-50-5

Molecular Formula: $C_{11}H_{10}N_2O$

Molecular Weight: 186.213

Accurate Mass: 186.079313

Percentage Composition: C 70.95%; H 5.41%; N 15.04%; O 8.59%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 166-167°

>>Derivative: 3-N-Ac; methosulfate

Physical Description: Yellow cryst.

Melting Point: Mp 171°

>>Derivative: N-Ph

Synonym(s): 3-Anilinoquinoline. *N*-Phenyl-3-quinolinamine, 9Cl

Molecular Formula: $C_{15}H_{12}N_2$

Molecular Weight: 220.273

Accurate Mass: 220.100048

Percentage Composition: C 81.79%; H 5.49%; N 12.72%

Physical Description: Needles (MeOH)

Melting Point: Mp 121-123°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **3**, 436B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 862D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1570D, (*ir*)

Mills, W.H. *et al.*, *J.C.S.*, 1910, **97**, 746

Bargellini, G. *et al.*, *Gazz. Chim. Ital.*, 1923, **53**, 601

Anet, R., *Can. J. Chem.*, 1959, **37**, 43, (*N-Ph*)