



>>Entry Name: 5-Aminoisoquinoline

Synonym(s): 5-Isoquinolinamine, 9Cl

CAS Registry Number: 1125-60-6

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: Pale-yellow cryst. (petrol)

Melting Point: Mp 128°

pKa Value: pK_a 5.57 (20°)

Aldrich: 13610-7

>>Derivative: Hydrochloride

Melting Point: Mp 270° (220° dec.)

>>Derivative: Methiodide

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 228°

>>Derivative: *N*-Ac

CAS Registry Number: 27461-33-2

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%

Melting Point: Mp 166°

>>Derivative: *N*-Benzoyl

Molecular Formula: $C_{16}H_{12}N_2O$

Molecular Weight: 248.284

Accurate Mass: 248.094963

Percentage Composition: C 77.40%; H 4.87%; N 11.28%; O 6.44%

Melting Point: Mp 158-159°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 879A, (*ir*)

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **3**, 459A, (*nmr*)

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Craig, J.J. *et al.*, *J.A.C.S.*, 1942, **64**, 783-784, (*synth, derivs*)

Ochiai, E. *et al.*, *Yakugaku Zasshi*, 1953, **73**, 666; *CA*, **48**, 7014, (*synth*)

Joseph, P.K. *et al.*, *J. Med. Chem.*, 1964, **7**, 801, (*synth*)

Potts, K.T. *et al.*, *J.O.C.*, 1986, **51**, 2011-2021, (*synth*)