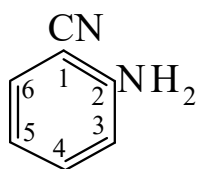




>>>Entry Name: 2-Aminobenzonitrile, 9CI

Synonym(s): Anthranilonitrile, 8CI. Anthranilic acid nitrile. *o*-Cyanoaniline



CAS Registry Number: 1885-29-6

Molecular Formula: C₇H₆N₂

Molecular Weight: 118.138

Accurate Mass: 118.053098

Percentage Composition: C 71.17%; H 5.12%; N 23.71%

Physical Description: Needles (petrol)

Melting Point: Mp 50-51°

Boiling Point: Bp 262-263°. Bp₁₁ 132-136°

pKa Value: pK_{a1} 0.77 (25°, 1% EtOH HCl aq.)

Aldrich: A8990-1

Fluka: 7001

>>Derivative: Hydrochloride

CAS Registry Number: 6944-57-6

Melting Point: Mp 197 dec.°

>>Derivative: *N*-Me

CAS Registry Number: 17583-40-3

Molecular Formula: C₈H₈N₂

Molecular Weight: 132.165

Accurate Mass: 132.068748

Percentage Composition: C 72.70%; H 6.10%; N 21.20%

Physical Description: Flakes (petrol)

Melting Point: Mp 72-73°

>>Derivative: *N,N*-Di-Me

CAS Registry Number: 20925-24-0

Molecular Formula: C₉H₁₀N₂

Molecular Weight: 146.191

Accurate Mass: 146.084398

Percentage Composition: C 73.94%; H 6.89%; N 19.16%

Physical Description: Liq.

Boiling Point: Bp₁₄ 137°. Bp₈ 122-124°

>>Derivative: *N*-Ac

CAS Registry Number: 25116-00-1

Molecular Formula: C₉H₈N₂O

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 134-135°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1511B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 444D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1408C, (*ir*)

Aldrich Library of IR Spectra, 2nd Ed., 983c, (*ir*)

Aldrich Library of NMR Spectra, **7**, 124A, (*pmr*)

Grammaticakis, P., *Bull. Soc. Chim. Fr.*, 1953, 207, (*uv*)

Bedford, G.R. *et al.*, *J.C.S.*, 1959, 1633, (*synth*)

Maquestiau, A. *et al.*, *Org. Mass Spectrom.*, 1974, **9**, 1188, (*ms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, APJ750