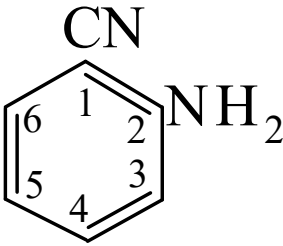




--Entry Name: 2-Aminobenzonitrile, 9C
Synonym(s): Anthranilonitrile, 9C; Anthranilic acid nitrile, o-Cyananiline



CAS Registry Number: 1885-29-6

Molecular Formula: C₇H₅N₂
Molecular Weight: 118.138
Accurate Mass: 118.03308
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°, Bp₁ 132-136°
pKa Value: pK_a 0.77 (25°, 1% EtOH HCl aq.)

Aldrich: A8990-1
Fluka: 701

--> Derivative: Hydrochloride

CAS Registry Number: 6944-57-6
Melting Point: Mp 197 dec.°

--> Derivative: N-Me

CAS Registry Number: 17583-40-3
Molecular Formula: C₈H₇N₂
Molecular Weight: 132.165
Accurate Mass: 132.06748
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: C₉H₉N₂
Molecular Weight: 146.191
Accurate Mass: 146.08498
Percentage Composition: C 73.94%; H 6.89%; N 19.16%
Physical Description: Liq
Boiling Point: Bp₁₄ 137°, Bp₁ 122-124°

--> Derivative: N-Ac

CAS Registry Number: 25116-00-1
Molecular Formula: C₈H₇N₂O
Molecular Weight: 160.175
Accurate Mass: 160.06363
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, (nmr)
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, AP7750