



>>Entry Name: Benzonitrile

Synonym(s): Phenyl cyanide. Cyanobenzene. Benzoic acid nitrile

CAS Registry Number: 100-47-0

PhCN

Molecular Formula: C₇H₅N

Molecular Weight: 103.123

Accurate Mass: 103.042199

Percentage Composition: C 81.53%; H 4.89%; N 13.58%

Source/Synthesis: Prod. comly. by vapour-phase cat. oxidn. of toluene/ammonia

Use/Importance: Powerful solvent, dissolves inorg. salts such as AgNO₃, FeCl₃ and some polymers. Used in industrial synth. of 2,4-Diamino-6-phenyl-1,3,5-triazine [FVZ84-O](#) used in coatings and moulding resins

Physical Description: Oil with almond-like odour

Melting Point: Fp -12.8°. Mp -13°

Boiling Point: Bp 191° (190.7°, 188°). Bp₁₀ 69°

Solubility: Misc. most org. solvs; spar. sol. hot H₂O (1% at 100°)

Density: d²⁰ 1.344

Refractive Index: n_D²⁰ 1.5289

Hazard & Toxicity: Fl. p. 72°. Skin irritant and vesicant. Adverse CNS effects (human and exp. data). LD₅₀ (rat, orl) 720 mg/kg; LD₅₀ (rat, skn) 1200 mg/kg

Aldrich: B895-9

Fluka: 12720

Sigma: B0657

>>Derivative: N-Oxide

Synonym(s): Benzonitrile N-oxide, 9CI

CAS Registry Number: 873-67-6

Molecular Formula: C₇H₅NO

Molecular Weight: 119.123

Accurate Mass: 119.037114

Percentage Composition: C 70.58%; H 4.23%; N 11.76%; O 13.43%

Use/Importance: Undergoes many cycloaddn. reacns.

Physical Description: Needles or oil with characteristic odour

Melting Point: Mp 15°

Other Data: Readily dimerises and isomerises

References:

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Denton, W.I. *et al.*, *Ind. Eng. Chem.*, 1950, **42**, 796, (*manuf*)

Huisgen, R. *et al.*, *Chem. Ber.*, 1972, **105**, 2805, (*N-oxide*)

Fauvet, G *et al.*, *Acta Cryst. B*, 1978, **34**, 1376, (*cryst struct*)

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