



>>Entry Name: Acetonitrile

Synonym(s): Methyl cyanide. Cyanomethane. Methanecarbonitrile. Ethanenitrile

CAS Registry Number: 75-05-8

Related CAS Registry Numbers(s): 2206-26-0 21438-99-3

H₃CCN

Molecular Formula: C₂H₃N

Molecular Weight: 41.052

Accurate Mass: 41.026549

Percentage Composition: C 58.52%; H 7.37%; N 34.12%

Use/Importance: Good solv. for inorganic salts and in org. synthesis. Polymer solvent. Used for sepn. of butadiene by extractive dist. CN⁽⁻⁾ is a metabolite and a thermal decomposition product.

Physical Description: Liq. with almond-ethereal odour

Melting Point: Mp -44.9°

Boiling Point: Bp 81.6°

Solubility: Misc. H₂O, most org. solvs., immisc. petrol

Density: d₄²⁰ 0.783

pKa Value: pK_a -4.3 (HClO₄)

Other Data: Forms constant-boiling mixt. with H₂O contg. 84% MeCN, Bp 76°

Hazard & Toxicity: Highly flammable, fl. p. 6° (oc), autoignition temp. 524°. Human fatalities reported following ingestion. LD₅₀ (rat, orl) 2730 mg/kg. Toxic effects, which may be delayed, are due to release of CN⁽⁻⁾. Exposure by skin absorption or inhalation causes headache, dizziness and nausea, and convulsions, coma and death at higher conc. OES: long-term 40 ppm; short-term 60 ppm

Aldrich: 31645-8

Fluka: 710

Sigma: P7216

Supelco: R80-1005

References:

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