



Synonym(s): 2-Propenenitrile, 9CI. Acrylonitrile. Vinyl cyanide. Cyanoethylene

CAS Registry Number: 107-13-1

Molecular Formula: C₃H₃N

Molecular Weight: 53.063

Accurate Mass: 53.026549

Percentage Composition: C 67.91%; H 5.70%; N 26.40%

Source/Synthesis: Manuf. from 1-Propene [BGX51-Z](#), oxygen and ammonia

Use/Importance: Undergoes free-radical initiated chain polym. Monomer for acrylic fibres, ABS resins, copolymers with styrene (SAN), etc. Cyanoethylating reagent. Used as an indicator in thermometric titrations. CN⁽⁻⁾ is a metabolite. Fumigant insecticide, now superseded. Important industrial chemical, 39th in order of volume for USA in 1994 (production 1.54 million tons/year)

Physical Description: Liq.

Melting Point: Mp -83°

Boiling Point: Bp 78°

Solubility: Sol. H₂O; misc. most org. solvs.

Density: d²⁰ 0.806

Refractive Index: n_D²⁰ 1.3911

Other Data: Vp 83 mmHg (20°). May polym. spontaneously, esp. in the absence of O₂ or on exposure to vis. light. Hydroquinone monomethyl ether is often added as an inhibitor. Q/e values for copolym., Q 0.48, e +1.23. Copolym. with vinyl chloride, r_{AN} 2.7, r_{VC} 0.04 (typical values, 60°), Q 0.60, e 1.20. Copolym. with vinylidene chloride, r_{VDC} 0.39 (33°), 0.37 (60°), r_{AN} 0.585 (33°), 0.91 (60°) (typical values)

Hazard & Toxicity: Highly flammable, fl. p. -5°, autoignition temp. 480°. Probable human carcinogen. Eye, skin and respiratory tract irritant. Adverse systemic effects on CNS, liver, kidneys, cardiovascular and gastrointestinal systems possible by skin absorption and other administration routes. Exp. carcinogen. Exp. reprod. and teratogenic effects. LD₅₀ (rat, orl) 78 mg/kg. LD₅₀ (rat, skn) 148 mg/kg. MEL: long-term 2 ppm (Sk)

Aldrich: 11021-3

Fluka: 1710

Supelco: R43-0030

>>**Derivative:** Anhydride

CAS Registry Number: 2051-76-5

Molecular Formula: C₆H₆O₃

Molecular Weight: 126.112

Accurate Mass: 126.031695

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Liq.

Boiling Point: Bp₃₅ 97°

Refractive Index: n_D²⁰ 1.4337

Other Data: Polym. to give linear polymers. Q/e values for copolym., Q 1.46, e +0.31

References: