



>>Entry Name: Cyanophosphonic acid, 9CI

$(\text{HO})_2\text{P}(\text{O})\text{CN}$

Molecular Formula: $\text{CH}_2\text{NO}_3\text{P}$

Molecular Weight: 107.005

Accurate Mass: 106.977231

Percentage Composition: C 11.22%; H 1.88%; N 13.09%; O 44.86%; P 28.95%

>>Derivative: Di-Et ester

CAS Registry Number: 2942-58-7

Molecular Formula: $\text{C}_5\text{H}_{10}\text{NO}_3\text{P}$

Molecular Weight: 163.113

Accurate Mass: 163.039831

Percentage Composition: C 36.82%; H 6.18%; N 8.59%; O 29.43%; P 18.99%

Use/Importance: Reagent for amide synth.

Physical Description: Oil

Boiling Point: Bp_{20} 103-104°

Hazard & Toxicity: LD_{50} (mus, scu) 25 mg/kg

Aldrich: 24673-5

Fluka: 28553

Sigma: D8520

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1490C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 919A, (ir)

Yamada, S. *et al.*, *Tetrahedron*, 1976, **32**, 2211, (synth, use)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 107, (use)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DJW800