



>>Entry Name: (Isocyanomethyl)phosphonic acid, 9Cl

$(\text{HO})_2\text{P}(\text{O})\text{CH}_2\text{NC}$

Molecular Formula: $\text{C}_2\text{H}_4\text{NO}_3\text{P}$

Molecular Weight: 121.032

Accurate Mass: 120.992881

Percentage Composition: C 19.85%; H 3.33%; N 11.57%; O 39.66%; P 25.59%

>>Derivative: Di-Et ester

Synonym(s): Diethyl (isocyanomethyl)phosphonate

CAS Registry Number: 41003-94-5

Molecular Formula: $\text{C}_6\text{H}_{12}\text{NO}_3\text{P}$

Molecular Weight: 177.139

Accurate Mass: 177.055481

Percentage Composition: C 40.68%; H 6.83%; N 7.91%; O 27.10%; P 17.49%

Use/Importance: A Wittig-Horner reagent for the synthesis of 1-isocyano-1-alkenes, (1-aminoalkyl)phosphonic acids and oxazoliny- and thiazolinyphosphonic acids

Physical Description: Liq.

Boiling Point: $\text{Bp}_{0.2}$ 90°

Aldrich: 35986-6

Fluka: 58833

Sigma: I0514

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1491B, (nmr)

Schöllkopf, U. *et al.*, *Annalen*, 1974, 44, (synth, ir, pmr, use)

Rachoń, J. *et al.*, *Annalen*, 1981, 709; 186; 1693, (props, use)

Rachoń, J., *Chimia*, 1983, **37**, 299; 1984, **38**, 114, (use)