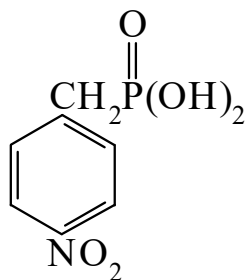




>>Entry Name: [(4-Nitrophenyl)methyl]phosphonic acid, 9Cl

Synonym(s): *p*-Nitrobenzylphosphonic acid



CAS Registry Number: 1205-62-5

Molecular Formula: C₇H₈NO₅P

Molecular Weight: 217.118

Accurate Mass: 217.014011

Percentage Composition: C 38.72%; H 3.71%; N 6.45%; O 36.84%; P 14.27%

Use/Importance: Alkaline phosphatase inhibitor. Antiviral agent

Physical Description: Cryst. (H₂O or 2-propanol/methylcyclohexane)

Melting Point: Mp 232-234° (225-226° dec.)

Boiling Point: Bp_{0.5} 183-187°

pKa Value: pK_{a1} 3.9; pK_{a2} 9.3 (80% EtOH aq.)

Rare Chemicals Library: S91580-7

>>Derivative: Di-Me ester

CAS Registry Number: 39980-20-6

Molecular Formula: C₉H₁₂NO₅P

Molecular Weight: 245.171

Accurate Mass: 245.045311

Percentage Composition: C 44.09%; H 4.93%; N 5.71%; O 32.63%; P 12.63%

Use/Importance: Reagent for Wittig-Horner reactions

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 75°

>>Derivative: Mono-Et ester

Synonym(s): Monoethyl (4-nitrobenzyl)phosphonate

CAS Registry Number: 72448-73-8

Molecular Formula: C₉H₁₂NO₅P

Molecular Weight: 245.171

Accurate Mass: 245.045311

Percentage Composition: C 44.09%; H 4.93%; N 5.71%; O 32.63%; P 12.63%

Physical Description: Solid

Melting Point: Mp 157.5-158.5°

>>Derivative: Mono-Et ester, cyclohexylammonium salt

Physical Description: Solid

Melting Point: Mp 260 dec.°

>>Derivative: Di-Et ester

CAS Registry Number: 2609-49-6

Molecular Formula: C₁₁H₁₆NO₅P

Molecular Weight: 273.225

Accurate Mass: 273.076611

Percentage Composition: C 48.36%; H 5.90%; N 5.13%; O 29.28%; P 11.34%

Use/Importance: Stereospecific Wittig reagent

Physical Description: Liq.

Boiling Point: Bp₃ 199-201°. Bp_{0.1} 148-153°

Refractive Index: n_D²⁵ 1.5220