



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

Synonym(s): *p*-Chlorobenzylphosphonic acid

CAS Registry Number: 39225-05-3

Structure by analogy with [(2-Chlorophenyl)methyl]phosphonic acid, [DQF71-H](#)

Molecular Formula: C₇H₈ClO₃P

Molecular Weight: 206.565

Accurate Mass: 205.989959

Percentage Composition: C 40.70%; H 3.90%; Cl 17.16%; O 23.24%; P 14.99%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 168-171°

>>Derivative: Di-Et ester

Synonym(s): Diethyl [(4-chlorophenyl)methyl]phosphonate

CAS Registry Number: 39225-17-7

Molecular Formula: C₁₁H₁₆ClO₃P

Molecular Weight: 262.672

Accurate Mass: 262.052559

Percentage Composition: C 50.30%; H 6.14%; Cl 13.50%; O 18.27%; P 11.79%

Use/Importance: Wittig-Horner reagent

Physical Description: Liq.

Boiling Point: Bp₃ 180°. Bp_{0.01} 137-138°

Refractive Index: n_D²⁰ 1.4940

>>Derivative: Dichloride

Molecular Formula: C₇H₆Cl₃OP

Molecular Weight: 243.456

Accurate Mass: 241.922183

Percentage Composition: C 34.53%; H 2.48%; Cl 43.69%; O 6.57%; P 12.72%

Physical Description: Liq.

Boiling Point: Bp_{1.2} 130-134°

References:

Williams, A. *et al.*, *J.C.S. Perkin 2*, 1973, 25, (*synth*)

Fresneda, P.M. *et al.*, *Synthesis*, 1981, 222, (*ester*)

Katritzky, A.R. *et al.*, *Org. Prep. Proced. Int.*, 1990, **22**, 209, (*synth, pmr, cmr*)

Nakamura, M. *et al.*, *J.C.S. Perkin 1*, 1994, 141, (*dichloride, synth*)