



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

Synonym(s): *p*-Methylbenzylphosphonic acid

CAS Registry Number: 13081-74-8

Molecular Formula: C<sub>8</sub>H<sub>11</sub>O<sub>3</sub>P

Molecular Weight: 186.147

Accurate Mass: 186.044582

Percentage Composition: C 51.62%; H 5.96%; O 25.79%; P 16.64%

Physical Description: Plates or needles (H<sub>2</sub>O)

Melting Point: Mp 189°

>>Derivative: Di-Et ester

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

CAS Registry Number: 3762-25-2

Molecular Formula: C<sub>12</sub>H<sub>19</sub>O<sub>3</sub>P

Molecular Weight: 242.254

Accurate Mass: 242.107182

Percentage Composition: C 59.50%; H 7.90%; O 19.81%; P 12.79%

Use/Importance: Wittig-Horner reagent

Physical Description: Pleasant smelling liq.

Boiling Point: Bp<sub>11</sub> 157-160°. Bp<sub>0.7</sub> 132-135°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4958

>>Derivative: Dichloride

Molecular Formula: C<sub>8</sub>H<sub>9</sub>Cl<sub>2</sub>OP

Molecular Weight: 223.038

Accurate Mass: 221.976806

Percentage Composition: C 43.08%; H 4.07%; Cl 31.79%; O 7.17%; P 13.89%

Physical Description: Liq.

Boiling Point: Bp<sub>2</sub> 130°

Density: d<sub>20</sub><sup>20</sup> 1.26

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5430

#### References:

Kosolapoff, G.M., *J.A.C.S.*, 1945, **67**, 2259, (*synth, ester*)

Mel'nikov, N.N. *et al.*, *Zh. Obshch. Khim.*, 1961, **31**, 3953; *J. Gen. Chem. USSR (Engl. Transl.)*, 1961, **31**, 3687, (*synth*)

Rafikov, S.R. *et al.*, *Zh. Obshch. Khim.*, 1964, **34**, 2230; *J. Gen. Chem. USSR (Engl. Transl.)*, 1964, **34**, 2241, (*synth, dichloride, ester*)

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

Ernst, L., *Org. Magn. Reson.*, 1977, **9**, 35, (*ester, cmr, nmr*)

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