



>>Entry Name: [(4-Chlorophenyl)methyl]triphenylphosphonium(1+), 9Cl

Synonym(s): (*p*-Chlorobenzyl)triphenylphosphonium(1+)

CAS Registry Number: 47522-13-4

Structure by analogy with [(2-Chlorophenyl)methyl]triphenylphosphonium(1+), [DSD21-W](#)

Molecular Formula: C₂₅H₂₁ClP⁽⁺⁾

Molecular Weight: 387.867

Accurate Mass: 387.106939

Percentage Composition: C 77.42%; H 5.46%; Cl 9.14%; P 7.99%

>>Derivative: Chloride

CAS Registry Number: 1530-39-8

Molecular Formula: C₂₅H₂₁Cl₂P

Molecular Weight: 423.32

Accurate Mass: 422.075791

Percentage Composition: C 70.93%; H 5.00%; Cl 16.75%; P 7.32%

Use/Importance: Source of ylide with MeONa or butyllithium

Melting Point: Mp 307-308° (270°)

Aldrich: 42458-7

>>Derivative: Chloride; hydrochloride

Physical Description: Solid

Melting Point: Mp 174 dec.°

>>Derivative: Bromide

CAS Registry Number: 51044-12-3

Molecular Formula: C₂₅H₂₁BrClP

Molecular Weight: 467.771

Accurate Mass: 466.045275

Percentage Composition: C 64.19%; H 4.52%; Br 17.08%; Cl 7.58%; P 6.62%

Use/Importance: Source of ylide with butyllithium

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 278-280°

>>Derivative: Ylide

Synonym(s): (4-Chlorophenylmethylene)triphenylphosphorane, 11Cl, 9Cl. (*p*-Chlorobenzylidene)triphenylphosphorane. Triphenylphosphonium (4-chlorophenyl)methylide, 11Cl

CAS Registry Number: 38897-99-3

Molecular Formula: C₂₅H₂₀ClP

Molecular Weight: 386.859

Accurate Mass: 386.099114

Percentage Composition: C 77.62%; H 5.21%; Cl 9.16%; P 8.01%

Use/Importance: Wittig reagent prepd. *in situ*

References:

- Leznoff, C.C. *et al.*, *Can. J. Chem.*, 1972, **50**, 528, (*chloride, use*)
LaMontagne, M.P., *J. Med. Chem.*, 1973, **16**, 68, (*chloride, use*)
Kendurkar, P.S. *et al.*, *Z. Naturforsch., B*, 1973, **28**, 475, (*bromide, pmr, use*)
Yamato, M. *et al.*, *Chem. Pharm. Bull.*, 1977, **25**, 706, (*bromide, use*)
Lumbroso, H. *et al.*, *J. Organomet. Chem.*, 1978, **161**, 347, (*ylide, struct*)
Kroppová, V. *et al.*, *Coll. Czech. Chem. Comm.*, 1981, **46**, 515, (*chloride, use*)
Kohle, R. *et al.*, *Z. Anorg. Allg. Chem.*, 1987, **551**, 179, (*synth, pmr, P-31 nmr*)