



>>Entry Name: Triphenyl-2-propenylphosphonium(1+), 9Cl

Synonym(s): Allyltriphenylphosphonium(1+), 8Cl

CAS Registry Number: 15912-76-2

Related CAS Registry Numbers(s): 80922-35-6

$\text{H}_2\text{C}=\text{CHCH}_2\text{P}^{(+)}\text{Ph}_3$

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{P}^{(+)}$

Molecular Weight: 303.363

Accurate Mass: 303.130262

Percentage Composition: C 83.14%; H 6.64%; P 10.21%

Other Data: PhLi or NaNH₂→ ylide

>>Derivative: Chloride

CAS Registry Number: 18480-23-4

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{ClP}$

Molecular Weight: 338.815

Accurate Mass: 338.099114

Percentage Composition: C 74.44%; H 5.95%; Cl 10.46%; P 9.14%

Physical Description: Cryst.

Melting Point: Mp 234° (229-231°)

Aldrich: 33351-4

Fluka: 6075

Rare Chemicals Library: S4640-0

>>Derivative: Bromide

CAS Registry Number: 1560-54-9

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{BrP}$

Molecular Weight: 383.267

Accurate Mass: 382.068598

Percentage Composition: C 65.81%; H 5.26%; Br 20.85%; P 8.08%

Physical Description: Cryst. ($\text{CH}_2\text{Cl}_2/\text{AcOH}$)

Melting Point: Mp 222-225°

Aldrich: A3660-3

Rare Chemicals Library: S4641-9

>>Derivative: Ylide

Synonym(s): Triphenyl-2-propenylidenephosphorane. Triphenylphosphonium 2-propenylide

CAS Registry Number: 15935-94-1

Molecular Formula: $\text{C}_{21}\text{H}_{19}\text{P}$

Molecular Weight: 302.355

Accurate Mass: 302.122437

Percentage Composition: C 83.42%; H 6.33%; P 10.24%

Use/Importance: Used in Wittig reactions

Physical Description: Red

References:

- Aldrich Library of ¹³C and ¹H FT NMR Spectra*, 1992, **2**, 1669A; 1669B, (*nmr*)
- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 545C, (*ir*)
- Keough, P. *et al.*, *J.O.C.*, 1964, **29**, 631, (*synth, props*)
- Fieser and Fieser's Reagents for Organic Synthesis*, Wiley, 1972, **5**, 7; **6**, 14, (*ylide, use*)
- Wood, G.W., *J.O.C.*, 1975, **40**, 636, (*ms*)
- Albright, T.A. *et al.*, *J.A.C.S.*, 1976, **98**, 6249, (*cmr, P-31 nmr*)
- Nesmeyanov, N.A. *et al.*, *J. Organomet. Chem.*, 1977, **129**, 41, (*tautom, pmr, P-31 nmr*)
- Padwa, A. *et al.*, *J.O.C.*, 1980, **45**, 4555, (*use*)
- Schlosser, M. *et al.*, *Chimia*, 1982, **36**, 396, (*ylide*)