



>>Entry Name: Hexyltriphenylphosphonium(1+), 9CI

CAS Registry Number: 47415-89-4

$\text{Ph}_3\text{P}^{(+)}(\text{CH}_2)_5\text{CH}_3$

Molecular Formula: $\text{C}_{24}\text{H}_{28}\text{P}^{(+)}$

Molecular Weight: 347.459

Accurate Mass: 347.192862

Percentage Composition: C 82.96%; H 8.12%; P 8.91%

Use/Importance: Treatment of salts with butyllithium yields the ylide, widely used in synth. of prostaglandins and pheromones

Hazard & Toxicity: Salts inhibit AChE activity in vertebrates and schistosomes

>>Derivative: Bromide

CAS Registry Number: 4762-26-9

Molecular Formula: $\text{C}_{24}\text{H}_{28}\text{BrP}$

Molecular Weight: 427.363

Accurate Mass: 426.131198

Percentage Composition: C 67.45%; H 6.60%; Br 18.70%; P 7.25%

Physical Description: Solid

Melting Point: Mp 201-204°

Aldrich: 30144-2

>>Derivative: Iodide

CAS Registry Number: 60106-53-8

Molecular Formula: $\text{C}_{24}\text{H}_{28}\text{IP}$

Molecular Weight: 474.363

Accurate Mass: 474.097335

Percentage Composition: C 60.77%; H 5.95%; I 26.75%; P 6.53%

Physical Description: Solid

Melting Point: Mp 130-131°. Mp 136-141°

Aldrich: 39197-2

>>Derivative: Ylide

Synonym(s): Hexyldenetriphenylphosphorane

Molecular Formula: $\text{C}_{24}\text{H}_{27}\text{P}$

Molecular Weight: 346.451

Accurate Mass: 346.185037

Percentage Composition: C 83.20%; H 7.85%; P 8.94%

Use/Importance: Reactive Wittig reagent used in prostaglandin synth. Prepd. *in situ*

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1668B, (*nmr*)

Hauser, C.F. *et al.*, *J.O.C.*, 1963, **28**, 372, (*bromide*)

Ohloff, G. *et al.*, *Helv. Chim. Acta*, 1973, **56**, 1176, (*ylide, use*)

Müller-Schwartz, D. *et al.*, *J. Chem. Ecol.*, 1976, **2**, 389, (*bromide, ir, ylide, use*)

Kowal, R. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 673, (*iodide*)

Bestmann, H.J. *et al.*, *Annalen*, 1981, 2117, (*ylide, use*)

Wilcockson, W.S. *et al.*, *Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1982, **72**, 101, (*pharmacol*)

Romanov, G.V. *et al.*, *Khim.-Farm. Zh.*, 1990, **24**, 23, (*synth*)