



>>Entry Name: Heptyltriphenylphosphonium(1+), 9Cl

CAS Registry Number: 78827-66-4

Related CAS Registry Numbers(s): 84787-37-1

$\text{Ph}_3\text{P}^{(+)}(\text{CH}_2)_6\text{CH}_3$

Molecular Formula: $\text{C}_{25}\text{H}_{30}\text{P}^{(+)}$

Molecular Weight: 361.486

Accurate Mass: 361.208512

Percentage Composition: C 83.07%; H 8.36%; P 8.57%

>>Derivative: Bromide

CAS Registry Number: 13423-48-8

Molecular Formula: $\text{C}_{25}\text{H}_{30}\text{BrP}$

Molecular Weight: 441.39

Accurate Mass: 440.146848

Percentage Composition: C 68.03%; H 6.85%; Br 18.10%; P 7.02%

Use/Importance: With $\text{NaN}(\text{SiMe}_3)_2$ gives the ylide

Physical Description: No phys. props. reported

Aldrich: 37753-8

>>Derivative: Iodide

CAS Registry Number: 59378-88-0

Molecular Formula: $\text{C}_{25}\text{H}_{30}\text{IP}$

Molecular Weight: 488.39

Accurate Mass: 488.112985

Percentage Composition: C 61.48%; H 6.19%; I 25.98%; P 6.34%

Use/Importance: NaOMe or MeLi yields the ylide

Physical Description: Solid

Melting Point: Mp 128-131°

>>Derivative: Ylide

Synonym(s): Heptylidenetriphenylphosphorane. Triphenylphosphonium heptylide

CAS Registry Number: 55367-56-1

Molecular Formula: $\text{C}_{25}\text{H}_{29}\text{P}$

Molecular Weight: 360.478

Accurate Mass: 360.200687

Percentage Composition: C 83.30%; H 8.11%; P 8.59%

Use/Importance: Wittig reagent employed in fatty acid synth. Prepd. *in situ*

References:

Hauser, C.F. *et al.*, *J.O.C.*, 1963, **38**, 372, (*bromide*)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1979, **112**, 1923, (*bromide, ylide, use*)

Adlof, R.O. *et al.*, *J. Labelled Compd. Radiopharm.*, 1981, **18**, 419, (*iodide, ylide, use*)

Wheaton, G.A. *et al.*, *J.O.C.*, 1983, **48**, 917, (*ylide, use*)