



>>Entry Name: (Cyanomethyl)triphenylphosphonium(1+), 9Cl

CAS Registry Number: 47181-92-0

Related CAS Registry Numbers(s): 15898-47-2

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

Molecular Formula: $\text{C}_{20}\text{H}_{17}\text{NP}^{(+)}$

Molecular Weight: 302.335

Accurate Mass: 302.109861

Percentage Composition: C 79.45%; H 5.67%; N 4.63%; P 10.24%

>>Derivative: Chloride

CAS Registry Number: 4336-70-3

Molecular Formula: $\text{C}_{20}\text{H}_{17}\text{ClNP}$

Molecular Weight: 337.787

Accurate Mass: 337.078713

Percentage Composition: C 71.12%; H 5.07%; Cl 10.50%; N 4.15%; P 9.17%

Physical Description: Cryst. (MeNO_2 or EtOH)

Melting Point: Mp 252°. Mp 278-279°

pKa Value: $\text{p}K_{\text{a}}$ 7.6

Other Data: Alkali yields the ylide Triphenylphosphoranylideneacetonitrile [GGM28-X](#)

Aldrich: 46493-7

Rare Chemicals Library: S63371-2

>>Derivative: Bromide

CAS Registry Number: 15898-47-2

Molecular Formula: $\text{C}_{20}\text{H}_{17}\text{BrNP}$

Molecular Weight: 382.239

Accurate Mass: 381.048197

Percentage Composition: C 62.85%; H 4.48%; Br 20.90%; N 3.66%; P 8.10%

Physical Description: Solid

Melting Point: Mp 255-257°

Rare Chemicals Library: S61668-0

>>Derivative: Iodide

CAS Registry Number: 77785-52-5

Molecular Formula: $\text{C}_{20}\text{H}_{17}\text{INP}$

Molecular Weight: 429.239

Accurate Mass: 429.014334

Percentage Composition: C 55.96%; H 3.99%; I 29.56%; N 3.26%; P 7.22%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 224-226°

References:

Trippett, S. *et al.*, *J.C.S.*, 1959, 3874, (*synth, props*)

Wagenknecht, J. *et al.*, *J.O.C.*, 1966, **31**, 3885

Albright, T.A. *et al.*, *J.A.C.S.*, 1975, **97**, 2942, (*P-31 nmr*)

Fluck, E. *et al.*, *Pure Appl. Chem.*, 1975, **44**, 373, (*pe*)

Tronchet, J.M.J. *et al.*, *Helv. Chim. Acta*, 1979, **62**, 1401, (*props*)

Kukhar', V.P. *et al.*, *Zh. Obshch. Khim.*, 1979, **49**, 1025; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 889, (*synth, ir, ylide*)

Kukhar', V.P. *et al.*, *Zh. Org. Khim.*, 1981, **17**, 180; *J. Org. Chem. USSR (Engl. Transl.)*, 1981, **17**, 161, (*iodide*)

Herconet, A. *et al.*, *Phosphorus Sulfur Relat. Elem.*, 1987, **29**, 111, (*bromide*)