



>>Entry Name: Triphenylphosphoranylideneacetonitrile, 9Cl, 8Cl

Synonym(s): Cyanomethylidenetriphenylphosphorane. Triphenylphosphoranylidenemethanenitrile. Triphenylphosphonium cyanomethylide

CAS Registry Number: 16640-68-9

Related CAS Registry Numbers(s): 105663-75-0

$\text{Ph}_3\text{P}=\text{CHCN}$

Molecular Formula:  $\text{C}_{20}\text{H}_{16}\text{NP}$

Molecular Weight: 301.327

Accurate Mass: 301.102036

Percentage Composition: C 79.72%; H 5.35%; N 4.65%; P 10.28%

Use/Importance: Wittig reagent

Physical Description: Cryst. ( $\text{C}_6\text{H}_6$ , petrol, EtOH, or  $\text{C}_6\text{H}_6$ /cyclohexane)

Melting Point: Mp 196-197°

Other Data: Forms an anion with  $\text{NaN}(\text{SiMe}_3)_2$

Aldrich: 28042-9

>>Derivative:  $\text{BH}_3$  adduct

Molecular Formula:  $\text{C}_{20}\text{H}_{19}\text{BNP}$

Molecular Weight: 315.161

Accurate Mass: 315.134816

Percentage Composition: C 76.22%; H 6.08%; B 3.43%; N 4.44%; P 9.83%

Physical Description: Solid

Other Data: Dec. at 156°

#### References:

Trippett, S., *J.C.S.*, 1959, 3874, (*synth, uv*)

Schiemenz, G.P. *et al.*, *Chem. Ber.*, 1961, **94**, 578, (*synth, props*)

Speziale, A.J. *et al.*, *J.A.C.S.*, 1963, **85**, 2790, (*props, nmr*)

Bestmann, H.J. *et al.*, *Annalen*, 1974, 1688, (*synth, ir*)

Corsaro, A. *et al.*, *J.C.S. Perkin 1*, 1977, 2154, (*prop, use*)

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

Wätjen, F. *et al.*, *Tet. Lett.*, 1982, **23**, 4741, (*props*)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1989, **122**, 1411, (*anion, props*)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1991, **124**, 199, (*borane adduct, ir, pmr, cmr, B-11 nmr, P-31 nmr*)