



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

Synonym(s): Triphenylphosphine dibromide. Bromotriphenylphosphonium bromide

CAS Registry Number: 1034-39-5

Ph₃PBr₂

Molecular Formula: C₁₈H₁₅Br₂P

Molecular Weight: 422.098

Accurate Mass: 419.967809

Percentage Composition: C 51.22%; H 3.58%; Br 37.86%; P 7.34%

General Statement: Ionises in soln. to Ph₃PBr⁽⁺⁾Br⁽⁻⁾

Use/Importance: Brominating agent, used to cleave ethers, esters and lactones to give alkyl bromides or acyl bromides. Converts phenols into acyl bromides, and deoxygenates epoxides. Brominates αβ-unsatd. ketones at the β-posn. Used in synth. of β-lactams. Converts ureas into carbodiimides and amides into ω-bromoalkanoic esters; benzoin into benzils

Physical Description: Large hygroscopic cryst.

Melting Point: Mp 260-270°

Solubility: Sol. DMF

Other Data: Rapidly dec. in air/moisture to give a mixed salt Mp 140-141°

Aldrich: 27094-6

Fluka: 93095

>>Derivative: Br₂ adduct

Synonym(s): Bromotriphenylphosphonium tribromide

Molecular Formula: C₁₈H₁₅Br₄P

Molecular Weight: 581.906

Accurate Mass: 577.844481

Percentage Composition: C 37.15%; H 2.60%; Br 54.93%; P 5.32%

Physical Description: Orange cryst.

Melting Point: Mp 117°

Other Data: Ionic

>>Derivative: I₂ adduct

Molecular Formula: C₁₈H₁₅Br₂I₂P

Molecular Weight: 675.907

Accurate Mass: 673.776755

Percentage Composition: C 31.99%; H 2.24%; Br 23.64%; I 37.55%; P 4.58%

Physical Description: Red needles

Melting Point: Mp 79°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1682C, (*nmr*)
Beveridge, A.D. *et al.*, *J.C.S.(A)*, 1966, 520, (*synth, struct*)
Levy, D. *et al.*, *J.O.C.*, 1967, **32**, 1265, (*use*)
Bestmann, H.J. *et al.*, *Annalen*, 1968, **718**, 24, (*use*)
Okada, I. *et al.*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1185, (*use*)
Anderson, A.G. *et al.*, *J.O.C.*, 1972, **37**, 626, (*use*)
Ho, T., *Synthesis*, 1972, 697, (*use*)
Appel, R. *et al.*, *Chem. Ber.*, 1973, **106**, 3450, (*use*)
Org. Synth., Coll. Vol., 5, 1973, 142; 249, (*use*)
De Wit, J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 281, (*use*)
Smisman, E.E. *et al.*, *J.O.C.*, 1975, **40**, 1640, (*use*)
Burton, D.J. *et al.*, *J.O.C.*, 1975, **40**, 3026, (*use*)
Machinek, R. *et al.*, *Synthesis*, 1975, 255, (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 645; **10**, 60; **7**, 109; **9**, 112; **13**, 333; **7**, 407; **12**, 554, (*use*)
Briggs, E.M. *et al.*, *Synthesis*, 1980, 295, (*use*)
Buono, G., *Synthesis*, 1981, 872, (*use*)
Piers, E. *et al.*, *Can. J. Chem.*, 1982, **60**, 210, (*use*)
Molina, P. *et al.*, *Synthesis*, 1982, 596, (*use*)
Cossio, F.P. *et al.*, *Tet. Lett.*, 1985, **26**, 3041, (*use*)
Aizpurua, J.M. *et al.*, *J.O.C.*, 1986, **51**, 4941, (*use*)
Vogt, H. *et al.*, *Z. Naturforsch., B*, 1993, **48**, 258, (*cryst struct*)