



>>Entry Name: (3-Methylbutyl)triphenylphosphonium(1+), 9CI

Synonym(s): Isopentyltriphenylphosphonium(1+). Isoamyltriphenylphosphonium(1+)

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

Molecular Formula: $\text{C}_{23}\text{H}_{26}\text{P}^{(+)}$

Molecular Weight: 333.432

Accurate Mass: 333.177212

Percentage Composition: C 82.85%; H 7.86%; P 9.29%

>>Derivative: Bromide

CAS Registry Number: 28322-40-9

Molecular Formula: $\text{C}_{23}\text{H}_{26}\text{BrP}$

Molecular Weight: 413.336

Accurate Mass: 412.115548

Percentage Composition: C 66.83%; H 6.34%; Br 19.33%; P 7.49%

Use/Importance: Treatment with butyllithium yields the ylide

Physical Description: Cryst. (MeOH/Et₂O or 2-propanol/EtOAc)

Melting Point: Mp 152-153° (138-140°)

Aldrich: 34777-9

Rare Chemicals Library: S62670-8

>>Derivative: Iodide

CAS Registry Number: 52710-37-9

Molecular Formula: $\text{C}_{23}\text{H}_{26}\text{IP}$

Molecular Weight: 460.337

Accurate Mass: 460.081685

Percentage Composition: C 60.01%; H 5.69%; I 27.57%; P 6.73%

Use/Importance: Ylide source

Physical Description: Solid

Melting Point: Mp 163-168°

Rare Chemicals Library: S94726-1

>>Derivative: Ylide

Synonym(s): 3-Methylbutyridenetriphenylphosphorane. Isopentyridenetriphenylphosphorane. Triphenylphosphonium 3-methylbutylide

CAS Registry Number: 39110-24-2

Molecular Formula: $\text{C}_{23}\text{H}_{25}\text{P}$

Molecular Weight: 332.424

Accurate Mass: 332.169387

Percentage Composition: C 83.10%; H 7.58%; P 9.32%

Use/Importance: Reactive Wittig reagent. Used in synth. of vitamin D₃

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1668A, (nmr)

Inhoffen, H.H. *et al.*, *Chem. Ber.*, 1959, **92**, 1959, (bromide, ylide, use)

Georgiou, P.E. *et al.*, *J.C.S. Perkin 1*, 1973, 888, (ylide, use)

Bogoslovskii, N.A. *et al.*, *Zh. Obshch. Khim.*, 1978, **48**, 908; *J. Gen. Chem. USSR (Engl. Transl.)*, 1978, **48**, 823, (bromide, ylide, use)

Fürst, A. *et al.*, *Helv. Chim. Acta*, 1982, **65**, 1499, (ylide, use)

Romanov, G.V. *et al.*, *Khim.-Farm. Zh.*, 1990, **24**, 28, (bromide, iodide, synth, P-31 nmr)