



>>Entry Name: (Triphenylphosphoranylidene)acetic acid, 9CI

CAS Registry Number: 15677-02-8

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

Molecular Formula: $\text{C}_{20}\text{H}_{17}\text{O}_2\text{P}$

Molecular Weight: 320.327

Accurate Mass: 320.096617

Percentage Composition: C 74.99%; H 5.35%; O 9.99%; P 9.67%

Use/Importance: Wittig reagent

>>Derivative: Me ester

>>Derivative: Et ester

>>Derivative: *tert*-Butyl ester

Synonym(s): *tert*-Butyl (triphenylphosphoranylidene)acetate

CAS Registry Number: 35000-38-5

Molecular Formula: $\text{C}_{24}\text{H}_{25}\text{O}_2\text{P}$

Molecular Weight: 376.434

Accurate Mass: 376.159217

Percentage Composition: C 76.58%; H 6.69%; O 8.50%; P 8.23%

Physical Description: Cryst. (EtOH/petrol)

Melting Point: Mp 154-155° (147°)

Aldrich: 36979-9

>>Derivative: Benzyl ester

Synonym(s): Benzyl (triphenylphosphoranylidene)acetate

CAS Registry Number: 86453-58-9

Molecular Formula: $\text{C}_{27}\text{H}_{23}\text{O}_2\text{P}$

Molecular Weight: 410.451

Accurate Mass: 410.143567

Percentage Composition: C 79.01%; H 5.65%; O 7.80%; P 7.55%

Physical Description: Cryst. (EtOH/petrol)

Melting Point: Mp 120°

>>Derivative: 2-Propenyl ester

CAS Registry Number: 104127-76-6

Molecular Formula: $\text{C}_{23}\text{H}_{21}\text{O}_2\text{P}$

Molecular Weight: 360.391

Accurate Mass: 360.127917

Percentage Composition: C 76.65%; H 5.87%; O 8.88%; P 8.59%

Melting Point: Mp 71-73°

Aldrich: 39441-6

>>Derivative: Nitrile

References:

- Aldrich Library of ^{13}C and ^1H FT NMR Spectra*, 1992, **2**, 1680B, (*nmr*)
Knorr, H. *et al.*, *Annalen*, 1977, 545, (*esters*)
Montgomery, J.A. *et al.*, *J.O.C.*, 1981, **46**, 594, (*use*)
Cook, M.P. *et al.*, *J.O.C.*, 1982, **47**, 4955, (*ester*)
Sanchi, R. *et al.*, *Indian J. Chem., Sect. A*, 1985, **24**, 1031, (*propyl ester, ir, pmr, complexes*)
Naden, F.W. *et al.*, *Chem. Ber.*, 1986, **119**, 1196, (*tert-butyl ester*)
Baldoli, C. *et al.*, *Synthesis*, 1987, 288, (*use*)