



>>Entry Name: (2-Oxoethyl)triphenylphosphonium(1+), 9Cl

Synonym(s): (Formylmethyl)triphenylphosphonium(1+), 8Cl

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

Molecular Formula: $\text{C}_{20}\text{H}_{18}\text{OP}^{(+)}$

Molecular Weight: 305.335

Accurate Mass: 305.109527

Percentage Composition: C 78.67%; H 5.94%; O 5.24%; P 10.14%

>>Derivative: Chloride

CAS Registry Number: 62942-43-2

Molecular Formula: $\text{C}_{20}\text{H}_{18}\text{ClOP}$

Molecular Weight: 340.788

Accurate Mass: 340.078379

Percentage Composition: C 70.49%; H 5.32%; Cl 10.40%; O 4.69%; P 9.09%

Use/Importance: Source of Triphenylphosphoranylideneacetaldehyde [GGL97-M](#)

Physical Description: Cryst. ($\text{CHCl}_3/\text{EtOAc}$)

Melting Point: Mp 212-213 dec.°

pKa Value: $\text{p}K_{\text{a}}$ 6.15 (25°, EtOH aq.)

Other Data: At pH10 in 10% EtOH aq., $t_{1/2} = 391 \pm 21$ hr. Exists mostly as *trans*-enol form in CHCl_3 , but as keto-form (100%) in MeOH

Aldrich: 30532-4

Fluka: 47718

>>Derivative: Bromide

CAS Registry Number: 19753-63-0

Molecular Formula: $\text{C}_{20}\text{H}_{18}\text{BrOP}$

Molecular Weight: 385.239

Accurate Mass: 384.047863

Percentage Composition: C 62.36%; H 4.71%; Br 20.74%; O 4.15%; P 8.04%

Use/Importance: Source of Triphenylphosphoranylideneacetaldehyde [GGL97-M](#)

Physical Description: Cryst. ($\text{CHCl}_3/\text{EtOAc}$)

Melting Point: Mp 191-192°

>>Derivative: Tetrafluoroborate

Molecular Formula: $\text{C}_{20}\text{H}_{18}\text{BF}_4\text{OP}$

Molecular Weight: 392.14

Accurate Mass: 392.112444

Percentage Composition: C 61.26%; H 4.63%; B 2.76%; F 19.38%; O 4.08%; P 7.90%

Physical Description: Solid

Melting Point: Mp 76-77°

>>Derivative: Ylide

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1677A, (*nmr*)

Trippett, S. *et al.*, *J.C.S.*, 1961, 1266, (*chloride, synth*)

Issleib, K. *et al.*, *Annalen*, 1968, **713**, 12, (*props*)

Devlin, C.J. *et al.*, *Tetrahedron*, 1972, **28**, 3501, (*bromide, synth, pmr, ir, ms, nmr*)

Nesmeyanov, N.A. *et al.*, *J. Organomet. Chem.*, 1977, **129**, 41, (*derivs, synth, tautom, ir, pmr*)

Wittig, G. *et al.*, *Annalen*, 1978, 362, (*use*)

Brittain, J.M. *et al.*, *Tetrahedron*, 1979, **35**, 1139, (*P-31 nmr*)