



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

Synonym(s): (Benzoylmethyl)triphenylphosphonium(1+). Phenacyltriphenylphosphonium, 8Cl

CAS Registry Number: 17638-55-0

Related CAS Registry Numbers(s): 1108-21-0 129972-88-9

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

Molecular Formula: $\text{C}_{26}\text{H}_{22}\text{OP}^{(+)}$

Molecular Weight: 381.433

Accurate Mass: 381.140827

Percentage Composition: C 81.87%; H 5.81%; O 4.19%; P 8.12%

>>Derivative: Chloride

CAS Registry Number: 1678-18-8

Molecular Formula: $\text{C}_{26}\text{H}_{22}\text{ClOP}$

Molecular Weight: 416.886

Accurate Mass: 416.109679

Percentage Composition: C 74.91%; H 5.32%; Cl 8.50%; O 3.84%; P 7.43%

Physical Description: Plates

Other Data: Forms Pd complex

>>Derivative: Bromide

CAS Registry Number: 6048-29-9

Molecular Formula: $\text{C}_{26}\text{H}_{22}\text{BrOP}$

Molecular Weight: 461.337

Accurate Mass: 460.079163

Percentage Composition: C 67.69%; H 4.81%; Br 17.32%; O 3.47%; P 6.71%

Use/Importance: $\text{Na}_2\text{CO}_3 \rightarrow$ ylide

Physical Description: Cryst. (EtOH/Et₂O or H₂O). Possibly exists in two cryst. forms

Melting Point: Mp 265-268 dec., 284-286° dec.°

pKa Value: pK_a 6.03 (25°, 66% EtOH aq.)

Other Data: Exists largely as keto tautomer in soln.

Aldrich: 15133-5

Rare Chemicals Library: S1650-1

>>Derivative: Iodide

CAS Registry Number: 6230-82-6

Molecular Formula: $\text{C}_{26}\text{H}_{22}\text{IOP}$

Molecular Weight: 508.337

Accurate Mass: 508.0453

Percentage Composition: C 61.43%; H 4.36%; I 24.96%; O 3.15%; P 6.09%

Use/Importance: NaOMe or Na₂CO₃ aq. $\rightarrow$ ylide. Reagent for synth. of ArCOC $\equiv$ CAr

Physical Description: Cryst. (H₂O)

Melting Point: Mp 259-260° (204-205°)

>>Derivative: Perchlorate

CAS Registry Number: 95407-68-4

Molecular Formula: $\text{C}_{26}\text{H}_{22}\text{ClO}_5\text{P}$

Molecular Weight: 480.883

Accurate Mass: 480.089339

Percentage Composition: C 64.94%; H 4.61%; Cl 7.37%; O 16.64%; P 6.44%

Physical Description: Solid

Melting Point: Mp 224-225°

>>Derivative: Ylide

References: