



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

Synonym(s): Acetonyltriphenylphosphonium(1+), 8Cl. Triphenylphosphonoacetone(1+)

CAS Registry Number: 17638-57-2

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

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{OP}^{(+)}$

Molecular Weight: 319.362

Accurate Mass: 319.125177

Percentage Composition: C 78.98%; H 6.31%; O 5.01%; P 9.70%

>>Derivative: Chloride

CAS Registry Number: 1235-21-8

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{ClOP}$

Molecular Weight: 354.815

Accurate Mass: 354.094029

Percentage Composition: C 71.09%; H 5.68%; Cl 9.99%; O 4.51%; P 8.73%

Physical Description: Hygroscopic prisms (EtOH/Et₂O) or cryst. (CHCl₃/Et₂O)

Melting Point: Mp 243-245°. Mp 235-236°

pKa Value: pK_{a1} 6.6 (80% EtOH aq.) pK_{a1} 17.8 (MeNO₂)

Other Data: Na₂CO₃ aq. yields the ylide

Aldrich: 15807-0

Fluka: 785

>>Derivative: Bromide

CAS Registry Number: 2236-01-3

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{BrOP}$

Molecular Weight: 399.266

Accurate Mass: 398.063513

Percentage Composition: C 63.17%; H 5.05%; Br 20.01%; O 4.01%; P 7.76%

Physical Description: Cryst. (CHCl₃/Et₂O or MeOH/EtOAc)

Melting Point: Mp 229°

pKa Value: pK_{a1} 7.5 (20°, H₂O)

Rare Chemicals Library: S94757-1

>>Derivative: Iodide

CAS Registry Number: 65602-18-8

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{IOP}$

Molecular Weight: 446.267

Accurate Mass: 446.02965

Percentage Composition: C 56.52%; H 4.52%; I 28.44%; O 3.59%; P 6.94%

Physical Description: Cryst. (H₂O or MeOH/EtOAc)

Melting Point: Mp 207-209°

>>Derivative: Tetrafluoroborate

CAS Registry Number: 55220-28-5

Molecular Formula: $\text{C}_{21}\text{H}_{20}\text{BF}_4\text{OP}$

Molecular Weight: 406.167

Accurate Mass: 406.128094

Percentage Composition: C 62.10%; H 4.96%; B 2.66%; F 18.71%; O 3.94%; P 7.63%

Physical Description: Cryst. (CHCl₃/Et₂O)

Melting Point: Mp 154°