



>>Entry Name: **Benzylphosphonic acid**, 8Cl

Synonym(s): (Phenylmethyl)phosphonic acid, 9Cl. Toluene- α -phosphonic acid

CAS Registry Number: 6881-57-8

PhCH₂P(O)(OH)₂

Molecular Formula: C₇H₉O₃P

Molecular Weight: 172.12

Accurate Mass: 172.028932

Percentage Composition: C 48.85%; H 5.27%; O 27.89%; P 18.00%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 173-175°

pKa Value: pK_{a1} 2.38; pK_{a2} 5.98 (25°,H₂O) pK_{a1} 1.8; pK_{a2} 7.4 (17°) pK_{a1} 6.2; pK_{a2} 13.9 (25°,MeOH)

>>Derivative: Mono-Me ester

Synonym(s): Methyl hydrogen benzylphosphonate

CAS Registry Number: 63581-66-8

Molecular Formula: C₈H₁₁O₃P

Molecular Weight: 186.147

Accurate Mass: 186.044582

Percentage Composition: C 51.62%; H 5.96%; O 25.79%; P 16.64%

Physical Description: Cryst. (heptane)

Melting Point: Mp 96-97°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl benzylphosphonate

CAS Registry Number: 773-47-7

Molecular Formula: C₉H₁₃O₃P

Molecular Weight: 200.174

Accurate Mass: 200.060232

Percentage Composition: C 54.00%; H 6.55%; O 23.98%; P 15.47%

Physical Description: Liq.

Boiling Point: Bp₂₅ 168-170°. Bp_{0.5} 110-112°

Rare Chemicals Library: S44313-1

>>Derivative: Mono-Et ester

Synonym(s): Ethyl hydrogen benzylphosphonate

CAS Registry Number: 18933-98-7

Molecular Formula: C₉H₁₃O₃P

Molecular Weight: 200.174

Accurate Mass: 200.060232

Percentage Composition: C 54.00%; H 6.55%; O 23.98%; P 15.47%

Physical Description: Cryst. (heptane)

Melting Point: Mp 63-65°

>>Derivative: Di-Et ester

see Diethyl benzylphosphonate, [DMS99-G](#)

>>Derivative: Dibutyl ester

Synonym(s): Dibutyl benzylphosphonate

CAS Registry Number: 3762-27-4

Molecular Formula: C₁₅H₂₅O₃P

Molecular Weight: 284.334

Accurate Mass: 284.154132

Percentage Composition: C 63.36%; H 8.86%; O 16.88%; P 10.89%

Physical Description: Liq.

Boiling Point: Bp₃ 140-143°