



>>Entry Name: [1,4-Phenylenebis(methylene)]bisphosphonic acid, 9Cl
Synonym(s): *p*-Xylylenediphosphonic acid. 1,4-Bis(phosphonomethyl)benzene

CAS Registry Number: 4546-06-9

Molecular Formula: C₈H₁₂O₆P₂
Molecular Weight: 266.127
Accurate Mass: 266.010914
Percentage Composition: C 36.11%; H 4.54%; O 36.07%; P 23.28%
Physical Description: Solid or cryst. (H₂O)
Melting Point: Mp 275-280 dec.°. Mp 321-323 dec.°

>>Derivative: Tetra-Me ester
Synonym(s): Tetramethyl [1,4-phenylenebis(methylene)]bisphosphonate

CAS Registry Number: 52577-04-5

Molecular Formula: C₁₂H₂₀O₆P₂
Molecular Weight: 322.234
Accurate Mass: 322.073514
Percentage Composition: C 44.73%; H 6.26%; O 29.79%; P 19.22%
Use/Importance: Used in Wittig-Horner reactions
Physical Description: Liq.

>>Derivative: Tetra-Et ester
Synonym(s): Tetraethyl [1,4-phenylenebis(methylene)]bisphosphonate

CAS Registry Number: 4546-04-7

Molecular Formula: C₁₆H₂₈O₆P₂
Molecular Weight: 378.341
Accurate Mass: 378.136114
Percentage Composition: C 50.79%; H 7.46%; O 25.37%; P 16.37%
Physical Description: Cryst. (C₆H₆/petrol)
Melting Point: Mp 73-74° (70-72°)
Boiling Point: Bp₇ 220°. Bp_{0.1} 203-206°

>>Derivative: Tetrapropyl ester
Synonym(s): Tetrapropyl [1,4-phenylenebis(methylene)]bisphosphonate

Molecular Formula: C₂₀H₃₆O₆P₂
Molecular Weight: 434.448
Accurate Mass: 434.198714
Percentage Composition: C 55.29%; H 8.35%; O 22.10%; P 14.26%
Physical Description: Solid
Melting Point: Mp 76-77°
Boiling Point: Bp₁ 240-245°

>>Derivative: Tetra-Ph ester
Synonym(s): Tetraphenyl [1,4-phenylenebis(methylene)]bisphosphonate

Molecular Formula: C₃₂H₂₈O₆P₂
Molecular Weight: 570.517
Accurate Mass: 570.136114
Percentage Composition: C 67.37%; H 4.95%; O 16.83%; P 10.86%
Physical Description: Cryst. (C₆H₆/Me₂CO)
Melting Point: Mp 172°