



>>Entry Name: 1,4-Benzenediacetic acid, 9CI

Synonym(s): 1,4-Bis(carboxymethyl)benzene. *p*-Phenylenediacetic acid. *p*-Xylene- ω,ω' -dicarboxylic acid

CAS Registry Number: 7325-46-4

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Needles (H₂O)

Melting Point: Mp 244° (236°)

Other Data: Several polyesters with glycols have been synth.

Aldrich: P2340-7

Fluka: 78470

>>Derivative: Di-Me ester

CAS Registry Number: 36076-25-2

Molecular Formula: C₁₂H₁₄O₄

Molecular Weight: 222.24

Accurate Mass: 222.08921

Percentage Composition: C 64.85%; H 6.35%; O 28.80%

Physical Description: Leaflets

Melting Point: Mp 56.5-57°

Boiling Point: Bp₁₅ 189-190°

>>Derivative: Di-Et ester

CAS Registry Number: 36076-26-3

Molecular Formula: C₁₄H₁₈O₄

Molecular Weight: 250.294

Accurate Mass: 250.12051

Percentage Composition: C 67.18%; H 7.25%; O 25.57%

Melting Point: Mp 59°

Rare Chemicals Library: S77450-2

>>Derivative: Dichloride

CAS Registry Number: 21062-19-1

Molecular Formula: C₁₀H₈Cl₂O₂

Molecular Weight: 231.077

Accurate Mass: 229.990134

Percentage Composition: C 51.98%; H 3.49%; Cl 30.68%; O 13.85%

Physical Description: Yellowish solid

>>Derivative: Diamide

CAS Registry Number: 30038-76-7

Molecular Formula: C₁₀H₁₂N₂O₂

Molecular Weight: 192.217

Accurate Mass: 192.089878

Percentage Composition: C 62.49%; H 6.29%; N 14.57%; O 16.65%

Physical Description: Leaflets or needles (H₂O)

Melting Point: Mp 290°

>>Derivative: Dinitrile

Synonym(s): 1,4-Benzenediacetonitrile. 1,4-Bis(cyanomethyl)benzene. α,α -Dicyano-*p*-xylene. *p*-Xylylene dicyanide

CAS Registry Number: 622-75-3

Molecular Formula: C₁₀H₈N₂

Molecular Weight: 156.187

Accurate Mass: 156.068748

Percentage Composition: C 76.90%; H 5.16%; N 17.94%

Physical Description: Needles (H₂O); prisms (Et₂O)

Melting Point: Mp 98°

Aldrich: P2380-6