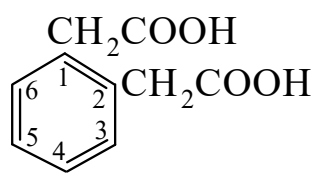




>>Entry Name: **1,2-Benzenediacetic acid**, 9CI

Synonym(s): 1,2-Bis(carboxymethyl)benzene. *o*-Phenylenediacetic acid. *o*-Xylene- ω,ω' -dicarboxylic acid



CAS Registry Number: 7500-53-0

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 or Et₂O)

Melting Point: Mp 151-152°

pKa Value: pK_a 3.95 (25°)

Aldrich: 13140-7

>>Derivative: Di-Me ester

CAS Registry Number: 19109-69-4

Molecular Formula: C₁₂H₁₄O₄

Molecular Weight: 222.24

Accurate Mass: 222.08921

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

Boiling Point: Bp_{0.18} 114°

Refractive Index: n_D²⁰ 1.5138

>>Derivative: Di-Et ester

CAS Registry Number: 17532-66-0

Molecular Formula: C₁₄H₁₈O₄

Molecular Weight: 250.294

Accurate Mass: 250.12051

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

Physical Description: Oil

Boiling Point: Bp₁₅ 185°

>>Derivative: Diamide

CAS Registry Number: 7500-54-1

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: Needles (H₂O)

Melting Point: Mp 198°

>>Derivative: Dinitrile

Synonym(s): 1,2-Benzenediacetonitrile. 1,2-Bis(cyanomethyl)benzene. α,α -Dicyano-*o*-xylene. *o*-Xylylene dicyanide

CAS Registry Number: 613-73-0

Molecular Formula: C₁₀H₈N₂

Molecular Weight: 156.187

Accurate Mass: 156.068748

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

Physical Description: Cryst. in two forms: prisms or needles (MeOH); prisms (EtOH)

Melting Point: Mp 18°. Mp 60° (dimorph.)

Aldrich: P2360-1

Fluka: 95750

References: