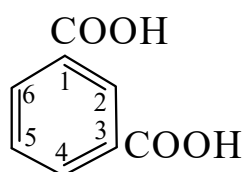




>>Entry Name: **1,3-Benzenedicarboxylic acid**, 9CI

Synonym(s): Isophthalic acid, 8CI. *m*-Phthalic acid



CAS Registry Number: 121-91-5

Related CAS Registry Numbers(s): 91816-63-6

Molecular Formula: C₈H₆O₄

Molecular Weight: 166.133

Accurate Mass: 166.02661

Percentage Composition: C 57.84%; H 3.64%; O 38.52%

Source/Synthesis: Manuf. industrially by catalytic oxidn. of 1,3-Dimethylbenzene [BLQ02-L](#)

Biological Source: Found in the rhizomes of *Iris versicolor*

Use/Importance: Monomer for polyesters, aramid fibres, and other polymers used in coatings, inks and packaging

Physical Description: Needles (H₂O or EtOH)

Melting Point: Mp 345-347°. Mp 348°

Solubility: Sl. sol. H₂O; sol. EtOH, AcOH; insol. C₆H₆, petrol; BERDY SOL: Sol. AcOH; fairly sol. EtOH; poorly sol. C₆H₆, H₂O

pKa Value: pK_{a1} 3.5; pK_{a2} 4.5 (25°)

Other Data: Subl.

Hazard & Toxicity: Eye irritant

Aldrich: I-1920-9

Fluka: 59200

Sigma: I5884

>>Derivative: Mono-Me ester

CAS Registry Number: 1877-71-0

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Melting Point: Mp 193°

>>Derivative: Mono-Et ester

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Melting Point: Mp 115-117°

>>Derivative: Di-Me ester

CAS Registry Number: 1459-93-4

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Use/Importance: Corrosion inhibitor for steel welds and used in manuf. of polyesters

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 67.8-68.3°

Boiling Point: Bp 282°. Bp₁₂ 124°

Hazard & Toxicity: Eye irritant

Aldrich: 19423-9

Fluka: 59220