



>>Entry Name: 1,2,4-Benzenetricarboxylic acid, 9CI

Synonym(s): Trimellitic acid

CAS Registry Number: 528-44-9

Molecular Formula: $C_9H_6O_6$

Molecular Weight: 210.143

Accurate Mass: 210.01644

Percentage Composition: C 51.44%; H 2.88%; O 45.68%

Source/Synthesis: Manuf. by oxidn. of 1,2,4-trimethylbenzene

Use/Importance: Used as a 2% aq. soln. for gravimetric detn. of Hf, Th, Zr; fluorescence detn. of Cu, V

Physical Description: Cryst. (AcOH or EtOH aq.)

Melting Point: Mp 229-230°. Mp 238°

Solubility: Sol. H_2O , Et_2O , EtOH

pKa Value: pK_{a1} 2.42; pK_{a2} 3.71; pK_{a3} 5.01 (25°, 0.1M KCl)

Hazard & Toxicity: LD₅₀ (mus, orl) 2500 mg/kg

Aldrich: B458-9

Fluka: 92119

Sigma: B6384

>>Derivative: 1-Me ester

CAS Registry Number: 13912-71-5

Molecular Formula: $C_{10}H_8O_6$

Molecular Weight: 224.17

Accurate Mass: 224.03209

Percentage Composition: C 53.58%; H 3.60%; O 42.82%

Physical Description: Cryst. in two forms

Melting Point: Mp 177°. Mp 203.5-205.5°

pKa Value: pK_{a1} 2.74; pK_{a2} 4.11 (25°)

>>Derivative: 2-Me ester

CAS Registry Number: 13940-95-9

Molecular Formula: $C_{10}H_8O_6$

Molecular Weight: 224.17

Accurate Mass: 224.03209

Percentage Composition: C 53.58%; H 3.60%; O 42.82%

Melting Point: Mp 208°

pKa Value: pK_{a1} 2.59; pK_{a2} 4

>>Derivative: 4-Me ester

CAS Registry Number: 29639-49-4

Molecular Formula: $C_{10}H_8O_6$

Molecular Weight: 224.17

Accurate Mass: 224.03209

Percentage Composition: C 53.58%; H 3.60%; O 42.82%

Physical Description: Leaflets (H_2O)

Melting Point: Mp 145-147°

pKa Value: pK_{a1} 2.54; pK_{a2} 4.96

>>Derivative: 1,2-Di-Me ester

CAS Registry Number: 54699-35-3

Molecular Formula: $C_{11}H_{10}O_6$

Molecular Weight: 238.196

Accurate Mass: 238.04774

Percentage Composition: C 55.47%; H 4.23%; O 40.30%

Physical Description: Needles (CS_2 , C_6H_6 or Et_2O /petrol)

Melting Point: Mp 115.5-117° (solidifies and remelts at 121°)

pKa Value: pK_a 3.47 (25°)