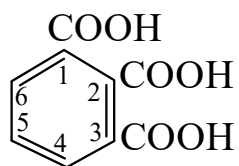




>>Entry Name: 1,2,3-Benzenetricarboxylic acid, 9CI

Synonym(s): Hemimellitic acid



CAS Registry Number: 569-51-7

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%

Physical Description: Needles (H_2O)

Melting Point: Mp 194-197 dec. $^{\circ}$

Density: d^{20}_4 1.546

pKa Value: pK_{a1} 2.62; pK_{a2} 3.82; pK_{a3} 5.51 (25 $^{\circ}$, 0.1M KCl)

Fluka: 51520

>>Derivative: Monohydrate

CAS Registry Number: 36362-97-7

Physical Description: Needles

Melting Point: Mp 223-224 $^{\circ}$

Aldrich: B420-1

Sigma: B1009

>>Derivative: Dihydrate

Physical Description: Plates

>>Derivative: Tri-Na salt

CAS Registry Number: 55680-81-4

Use/Importance: Used for fluorescence detn. of Cu, V

>>Derivative: 2-Me ester

CAS Registry Number: 31158-53-9

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 203-205 $^{\circ}$

>>Derivative: 1,3-Di-Me ester

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%

Melting Point: Mp 148-150 $^{\circ}$

>>Derivative: Tri-Me ester

CAS Registry Number: 2672-57-3

Molecular Formula: $C_{12}H_{12}O_6$

Molecular Weight: 252.223

Accurate Mass: 252.06339

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Plates (MeOH)

Melting Point: Mp 102 $^{\circ}$