



>>Entry Name: 3,6-Dihydroxy-1,2-benzenedicarboxylic acid, 9CI

Synonym(s): 3,6-Dihydroxyphthalic acid, 8CI. Hydroquinone-2,3-dicarboxylic acid

CAS Registry Number: 3786-46-7

Structure by analogy with 2,3-Dihydroxy-1,4-benzenedicarboxylic acid, [DZP44-K](#)

Molecular Formula: C₈H₆O₆

Molecular Weight: 198.132

Accurate Mass: 198.01644

Percentage Composition: C 48.50%; H 3.05%; O 48.45%

Physical Description: Yellow-green needles (H₂O)

Melting Point: Mp 224-225 dec.°

Rare Chemicals Library: S91947-0

>>Derivative: Di-Me ester

CAS Registry Number: 7474-92-2

Molecular Formula: C₁₀H₁₀O₆

Molecular Weight: 226.185

Accurate Mass: 226.04774

Percentage Composition: C 53.10%; H 4.46%; O 42.44%

Physical Description: Needles (H₂O)

Melting Point: Mp 141-142°

>>Derivative: Di-Et ester

CAS Registry Number: 15460-24-9

Molecular Formula: C₁₂H₁₄O₆

Molecular Weight: 254.239

Accurate Mass: 254.07904

Percentage Composition: C 56.69%; H 5.55%; O 37.76%

Melting Point: Mp 89°

>>Derivative: Dinitrile

Synonym(s): 2,3-Dicyano-1,4-benzenediol. 2,3-Dicyanohydroquinone. 3,6-Dihydroxy-1,2-benzenedicarbonitrile, 9CI

CAS Registry Number: 4733-50-0

Molecular Formula: C₈H₄N₂O₂

Molecular Weight: 160.132

Accurate Mass: 160.027278

Percentage Composition: C 60.01%; H 2.52%; N 17.49%; O 19.98%

Use/Importance: Used as 1% EtOH soln. as fluorescent acid-base indicator (pH range: 5.8-8.2; colour change: blue → green)

Physical Description: Yellow leaflets + 2H₂O

Solubility: Sol. alkalis, EtOH, Et₂O, Me₂CO; spar. sol. H₂O, C₆H₆, CHCl₃

Other Data: Blackens at 230°

Aldrich: 14113-5

Fluka: 36611

Sigma: D0554

>>Derivative: Di-Me ether

Synonym(s): 3,6-Dimethoxy-1,2-benzenedicarboxylic acid. 3,6-Dimethoxyphthalic acid

CAS Registry Number: 64019-77-8

Molecular Formula: C₁₀H₁₀O₆

Molecular Weight: 226.185

Accurate Mass: 226.04774

Percentage Composition: C 53.10%; H 4.46%; O 42.44%

Physical Description: Yellow prisms + 1H₂O (H₂O)

Melting Point: Mp 183-186 dec.°