



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

Synonym(s): 4-Hydroxyphthalic acid

CAS Registry Number: 610-35-5

Molecular Formula: C₈H₆O₅

Molecular Weight: 182.132

Accurate Mass: 182.021525

Percentage Composition: C 52.76%; H 3.32%; O 43.92%

Melting Point: Mp 312°

>>Derivative: Di-Me ester

CAS Registry Number: 22479-95-4

Molecular Formula: C₁₀H₁₀O₅

Molecular Weight: 210.186

Accurate Mass: 210.052825

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

Melting Point: Mp 105.5°

>>Derivative: Dinitrile

Synonym(s): 4-Hydroxyphthalonitrile. 3,4-Dicyanophenol

CAS Registry Number: 30757-50-7

Molecular Formula: C₈H₄N₂O

Molecular Weight: 144.132

Accurate Mass: 144.032363

Percentage Composition: C 66.67%; H 2.80%; N 19.44%; O 11.10%

Use/Importance: Intermed. in phthalocyanine synth.

Physical Description: Solid (AcOH)

Melting Point: Mp 218° (208-210°)

>>Derivative: Me ether

Synonym(s): 4-Methoxy-1,2-benzenedicarboxylic acid

CAS Registry Number: 1885-13-8

Molecular Formula: C₉H₈O₅

Molecular Weight: 196.159

Accurate Mass: 196.037175

Percentage Composition: C 55.11%; H 4.11%; O 40.78%

Physical Description: Cryst. (EtOH/C₆H₆)

Melting Point: Mp 160-162°

pK_a Value: pK_{a1} 2.67; pK_{a2} 5.16 (25°, 0.1M KNO₃)

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>>Derivative: Ph ether, dinitrile

Synonym(s): 1,2-Dicyano-4-phenoxybenzene

CAS Registry Number: 38791-62-7

Molecular Formula: C₁₄H₈N₂O

Molecular Weight: 220.23

Accurate Mass: 220.063663

Percentage Composition: C 76.35%; H 3.66%; N 12.72%; O 7.26%

Melting Point: Mp 100-101°

References:

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Bradsher, C.K. *et al.*, *J.O.C.*, 1961, **26**, 3278, (*synth*, *Me ether*)

Danishofsky, S. *et al.*, *J.A.C.S.*, 1974, **96**, 7807, (*synth*)

Carter, J.E. *et al.*, *J. Pharm. Sci.*, 1977, **66**, 546, (*synth*, *pmr*)

Ustinov, V.A. *et al.*, *Zh. Org. Khim.*, 1979, **15**, 1775; *J. Org. Chem. USSR (Engl. Transl.)*, 1979, **15**, 1595, (*nitrile*)

Wöhrle, D. *et al.*, *Synth. Commun.*, 1989, **19**, 3231, (*nitrile*)

Heffner, R.J. *et al.*, *Synth. Commun.*, 1991, **21**, 2231, (*synth*, *ir*, *pmr*, *ester*)