



**>>Entry Name: 4-Hydroxy-2-methylbenzoic acid**

**Synonym(s):** 4-Hydroxy-*o*-toluic acid. *m*-Cresol-4-carboxylic acid. 4,2-Cresotic acid

**CAS Registry Number:** 578-39-2

**Molecular Formula:** C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>

**Molecular Weight:** 152.149

**Accurate Mass:** 152.047345

**Percentage Composition:** C 63.15%; H 5.30%; O 31.55%

**Physical Description:** Needles + ½ H<sub>2</sub>O (H<sub>2</sub>O)

**Melting Point:** Mp 177-178° (anhyd.)

**pKa Value:** p*K*<sub>a1</sub> 4.71 (20°, 1% EtOH)

**>>Derivative:** Et ester

**CAS Registry Number:** 57081-00-2

**Molecular Formula:** C<sub>10</sub>H<sub>12</sub>O<sub>3</sub>

**Molecular Weight:** 180.203

**Accurate Mass:** 180.078645

**Percentage Composition:** C 66.65%; H 6.71%; O 26.64%

**Physical Description:** Needles (petrol)

**Melting Point:** Mp 98°

**Boiling Point:** Bp 300°

**>>Derivative:** Nitrile

**Synonym(s):** 4-Hydroxy-2-methylbenzonitrile. 4-Cyano-3-methylphenol

**Molecular Formula:** C<sub>8</sub>H<sub>7</sub>NO

**Molecular Weight:** 133.149

**Accurate Mass:** 133.052764

**Percentage Composition:** C 72.17%; H 5.30%; N 10.52%; O 12.02%

**Melting Point:** Mp 100-101°

**>>Derivative:** Me ether

**Synonym(s):** 4-Methoxy-2-methylbenzoic acid

**CAS Registry Number:** 6245-57-4

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>O<sub>3</sub>

**Molecular Weight:** 166.176

**Accurate Mass:** 166.062995

**Percentage Composition:** C 65.05%; H 6.07%; O 28.88%

**Physical Description:** Needles (H<sub>2</sub>O)

**Melting Point:** Mp 176°

**Boiling Point:** Bp<sub>16</sub> 143°

**pKa Value:** p*K*<sub>a1</sub> 4.54 (20°, 1% EtOH)

**References:**

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Rosenmund, K.W., *Annalen*, 1928, **460**, 56  
King, C. *et al.*, *J.A.C.S.*, 1945, **67**, 2089  
Beer, R. *et al.*, *J.C.S.*, 1949, 885, (*nitrile*)  
Fujio, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127, (*pmr, ester*)  
Comins, D.L. *et al.*, *J.O.C.*, 1986, **51**, 3566, (*synth, deriv*)  
Hauser, F.M. *et al.*, *Synthesis*, 1987, 723, (*deriv, synth, ir, pmr, ms*)  
Collins, M.J. *et al.*, *Aust. J. Chem.*, 1992, **45**, 1119, (*ms, pmr, nitrile*)  
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