



>>Entry Name: 4-Hydroxy-3-methylbenzoic acid

Synonym(s): 4-Hydroxy-*m*-toluic acid. *o*-Cresol-4-carboxylic acid. 4,3-Cresotic acid

CAS Registry Number: 499-76-3

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

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

Physical Description: Needles + ½H₂O (H₂O)

Melting Point: Mp 174-175° (anhyd.)

pKa Value: p*K*_{a1} 4.68 (20°, 1% EtOH)

>>Derivative: Et ester

CAS Registry Number: 69747-21-3

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

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

Physical Description: Needles (petrol/C₆H₆)

Melting Point: Mp 98-99°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-methylphenol

CAS Registry Number: 15777-70-5

Molecular Formula: C₈H₇NO

Molecular Weight: 133.149

Accurate Mass: 133.052764

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

Physical Description: Needles (H₂O)

Melting Point: Mp 93°

>>Derivative: Ac

CAS Registry Number: 23298-84-2

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 75-76°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-3-methylbenzoic acid

CAS Registry Number: 6880-04-2

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

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

Physical Description: Needles (H₂O)

Melting Point: Mp 196-197°

pKa Value: p*K*_{a1} 4.35 (20°, 1% EtOH)

References:

Gattermann, L. *et al.*, *Annalen*, 1888, **244**, 65, (*synth*)

King, C. *et al.*, *J.A.C.S.*, 1945, **67**, 2089, (*synth*)

Chattopadhyaya, M.C. *et al.*, *Indian J. Chem.*, 1971, **9**, 490

Fujio, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127, (*pmr*)

Schow, S.R. *et al.*, *J.A.C.S.*, 1986, **108**, 2662, (*deriv, synth, pmr*)