



>>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: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

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

Physical Description: Needles + ½ H₂O (H₂O)

Melting Point: Mp 177-178° (anhyd.)

pKa Value: p*K*_{a1} 4.71 (20°, 1% EtOH)

>>Derivative: Et ester

CAS Registry Number: 57081-00-2

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)

Melting Point: Mp 98°

Boiling Point: Bp 300°

>>Derivative: Nitrile

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

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%

Melting Point: Mp 100-101°

>>Derivative: Me ether

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

CAS Registry Number: 6245-57-4

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 176°

Boiling Point: Bp₁₆ 143°

pKa Value: p*K*_{a1} 4.54 (20°, 1% EtOH)

References:

- Gomberg, M. *et al.*, *J.A.C.S.*, 1917, **39**, 1679
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*)
Bennetau, B. *et al.*, *J.C.S. Perkin 1*, 1995, 1265, (*Me ether, synth, pmr, cmr*)