



>>Entry Name: 3-Hydroxy-4-iodobenzoic acid, 9CI

CAS Registry Number: 58123-77-6

Molecular Formula: C₇H₅IO₃

Molecular Weight: 264.019

Accurate Mass: 263.928343

Percentage Composition: C 31.85%; H 1.91%; I 48.07%; O 18.18%

Physical Description: Needles

Melting Point: Mp 226-230°

pKa Value: pK_a 5.37 (25°, 50% EtOH aq.)

>>Derivative: Me ester

CAS Registry Number: 157942-12-6

Molecular Formula: C₈H₇IO₃

Molecular Weight: 278.046

Accurate Mass: 277.943993

Percentage Composition: C 34.56%; H 2.54%; I 45.64%; O 17.26%

Physical Description: Solid

Melting Point: Mp 145-148°

>>Derivative: Ac

Molecular Formula: C₉H₇IO₄

Molecular Weight: 306.056

Accurate Mass: 305.938908

Percentage Composition: C 35.32%; H 2.31%; I 41.46%; O 20.91%

Physical Description: Leaflets

Melting Point: Mp 203°

>>Derivative: Anilide

CAS Registry Number: 19503-67-4

Molecular Formula: C₁₃H₁₀INO₂

Molecular Weight: 339.132

Accurate Mass: 338.975627

Percentage Composition: C 46.04%; H 2.97%; I 37.42%; N 4.13%; O 9.44%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 188°

>>Derivative: Me ether

Synonym(s): 4-Iodo-3-methoxybenzoic acid. 4-Iodo-*m*-anisic acid

Molecular Formula: C₈H₇IO₃

Molecular Weight: 278.046

Accurate Mass: 277.943993

Percentage Composition: C 34.56%; H 2.54%; I 45.64%; O 17.26%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 210-213°

References:

King, L.C. *et al.*, *J.A.C.S.*, 1945, **67**, 2089-2091, (*synth*)

Frank, H.R. *et al.*, *J.A.C.S.*, 1948, **70**, 2314-2320, (*synth*)

Cockerill, G.S. *et al.*, *J.C.S. Perkin I*, 1995, 1103-1113, (*Me ester, synth, ir, pmr, cmr*)

Pilling, R.J. *et al.*, *J.C.S. Perkin I*, 1999, 2077-2086, (*synth, pmr*)