



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

Synonym(s): 3-Iodo-*p*-toluic acid

CAS Registry Number: 82998-57-0

Molecular Formula: C₈H₇IO₂

Molecular Weight: 262.047

Accurate Mass: 261.949078

Percentage Composition: C 36.67%; H 2.69%; I 48.43%; O 12.21%

Melting Point: Mp 208-209°

Aldrich: 27885-8

>>Derivative: Me ester

Molecular Formula: C₉H₉IO₂

Molecular Weight: 276.073

Accurate Mass: 275.964728

Percentage Composition: C 39.16%; H 3.29%; I 45.97%; O 11.59%

Melting Point: Mp 28°

Boiling Point: Bp₅₂ 194°

>>Derivative: Et ester

Molecular Formula: C₁₀H₁₁IO₂

Molecular Weight: 290.1

Accurate Mass: 289.980378

Percentage Composition: C 41.40%; H 3.82%; I 43.75%; O 11.03%

Boiling Point: Bp₁₇₅ 242°

>>Derivative: Chloride

Synonym(s): 3-Iodo-4-methylbenzoyl chloride

CAS Registry Number: 52107-98-9

Molecular Formula: C₈H₆ClIO

Molecular Weight: 280.492

Accurate Mass: 279.91519

Percentage Composition: C 34.26%; H 2.16%; Cl 12.64%; I 45.24%; O 5.70%

Boiling Point: Bp_{1.3} 110°

>>Derivative: Amide

Synonym(s): 3-Iodo-4-methylbenzamide

Molecular Formula: C₈H₈INO

Molecular Weight: 261.062

Accurate Mass: 260.965062

Percentage Composition: C 36.81%; H 3.09%; I 48.61%; N 5.37%; O 6.13%

Melting Point: Mp 167°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-iodo-1-methylbenzene. 4-Cyano-2-iodotoluene

CAS Registry Number: 42872-79-7

Molecular Formula: C₈H₆IN

Molecular Weight: 243.047

Accurate Mass: 242.954497

Percentage Composition: C 39.53%; H 2.49%; I 52.21%; N 5.76%

Melting Point: Mp 57-58°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1103B, (*nmr*)

Kenner, J. *et al.*, *J.C.S.*, 1913, **103**, 232, (*synth*)

Gore, P.H. *et al.*, *J.C.S. Perkin 1*, 1973, 2940, (*synth*)

Hands, D. *et al.*, *J. Het. Chem.*, 1986, **23**, 1333, (*synth*)