



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

Synonym(s): 4-Iodo-*m*-toluic acid

CAS Registry Number: 52107-87-6

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 223-224°

>>Derivative: Me ester

CAS Registry Number: 5471-81-8

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 58-60°

Boiling Point: Bp_{0.35} 103-106°

>>Derivative: Chloride

CAS Registry Number: 52107-94-5

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_{0.3} 96-98°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-1-iodo-2-methylbenzene. 5-Cyano-2-iodotoluene

CAS Registry Number: 42872-85-5

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 76-77°

References:

Chardonens, L. *et al.*, *Helv. Chim. Acta*, 1970, **53**, 1083, (*synth*)

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