



>>Entry Name: 2-Iodo-5-methylbenzoic acid, 9CI

Synonym(s): 6-Iodo-*m*-toluic acid

CAS Registry Number: 52548-14-8

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 123-124°

pKa Value: p*K*_{a1} 2.95 (20°, 1% EtOH)

>>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%

Boiling Point: Bp_{0.6} 104-105°

>>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: Bp_{0.5} 118-122°

>>Derivative: Chloride

CAS Registry Number: 52107-96-7

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} 95-96°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-1-iodo-4-methylbenzene. 3-Cyano-4-iodotoluene

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 53-54°

References:

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

Bonilha, J.B.S. *et al.*, *Chem. Ber.*, 1978, **111**, 2510, (*synth*, *ir*, *nmr*)

Katritzky, A.R. *et al.*, *Org. Prep. Proced. Int.*, 1989, **21**, 157, (*synth*)

Moss, R.A. *et al.*, *J.O.C.*, 1990, **55**, 2064, (*synth*)