



>>Entry Name: 1-Iodo-4-methylbenzene

Synonym(s): 4-Iodotoluene

CAS Registry Number: 624-31-7

Molecular Formula: C₇H₇I

Molecular Weight: 218.037

Accurate Mass: 217.959248

Percentage Composition: C 38.56%; H 3.24%; I 58.20%

Physical Description: Leaves (EtOH)

Melting Point: Mp 36-37° (24°)

Boiling Point: Bp 211°. Bp₂₅ 100°

Density: d₄⁴⁰ 1.678

Other Data: Sublimes

Hazard & Toxicity: Explodes above 200°

Aldrich: 20655-5

Fluka: 58110

>>Derivative: Dichloride

Molecular Formula: C₇H₇Cl₂I

Molecular Weight: 288.942

Accurate Mass: 287.896952

Percentage Composition: C 29.10%; H 2.44%; Cl 24.54%; I 43.92%

Melting Point: Mp 100°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 90B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 991B, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 909B, (ir)

Nichol, J.C. *et al.*, *J.A.C.S.*, 1945, **67**, 1307

Choong-Tai Ahn *et al.*, *Acta Cryst. B*, 1972, **28**, 2152, (cryst struct)

Felix, G. *et al.*, *Angew. Chem.*, 1977, **89**, 502, (synth)

Shapiro, B.L. *et al.*, *J. Phys. Chem. Ref. Data*, 1977, **6**, 919, (nmr)

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