



>>Entry Name: 3-Methylthiophene

Synonym(s): β -Thiotolene

CAS Registry Number: 616-44-4

Molecular Formula: C₅H₆S

Molecular Weight: 98.168

Accurate Mass: 98.01902

Percentage Composition: C 61.18%; H 6.16%; S 32.66%

Source/Synthesis: Found in coal tar

Melting Point: Mp -69°

Boiling Point: Bp 115°

Density: d²⁰ 1.025

Refractive Index: n_D²⁰ 1.5204

Hazard & Toxicity: LD₅₀ (mus, orl) 1800 mg/kg

Aldrich: M8440-2

Fluka: 69370

Sigma: M8014

References:

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Reddy, G.S. *et al.*, *J.A.C.S.*, 1961, **83**, 5020, (*nmr*)

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Mathis, C.T. *et al.*, *J. Phys. Chem.*, 1964, **68**, 571, (*pmr*)

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Minoru, A., *J. Mol. Spectrosc.*, 1972, **43**, 226, (*ir*)

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