



>>Entry Name: 4,5-Dimethylthiazole

ENTRY UNDER REVIEW

Synonym(s): FEMA 3274

CAS Registry Number: 3581-91-7

Type of Compound Code(s): WE9999

Structure by analogy with 2,4-Dimethylthiazole, [FWX44-Z](#)

Molecular Formula: C₅H₇NS

Molecular Weight: 113.183

Accurate Mass: 113.029919

Percentage Composition: C 53.06%; H 6.23%; N 12.38%; S 28.33%

Melting Point: Mp 83-84°

Boiling Point: Bp 158°. Bp₄₇ 75°

Solubility: Sol. Et₂O, EtOH

pK_a Value: pK_a 3.73 (25°)

Aldrich: 21917-7

>>Derivative: Picrate

Physical Description: Cryst. (EtOH)

Melting Point: Mp 186-187°

>>Derivative: N-Oxide

Molecular Formula: C₅H₇NOS

Molecular Weight: 129.182

Accurate Mass: 129.024834

Percentage Composition: C 46.49%; H 5.46%; N 10.84%; O 12.39%; S 24.82%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 116-117°

>>Derivative: N-Me

Synonym(s): 3,4,5-Trimethylthiazolium

Molecular Formula: C₆H₁₀NS⁽⁺⁾

Molecular Weight: 128.218

Accurate Mass: 128.053394

Percentage Composition: C 56.21%; H 7.86%; N 10.92%; S 25.01%

Physical Description: Cryst. (EtOH) (as iodide)

Melting Point: Mp 223-223.5 dec.° (iodide)

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 109C, (*nmr*)

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Buchman, E.R. *et al.*, *J.O.C.*, 1941, **6**, 764

Kurkijy, R.P. *et al.*, *J.A.C.S.*, 1952, **74**, 5778, (*synth*)

Haag, A. *et al.*, *Org. Mass Spectrom.*, 1976, **11**, 511, (*ms*)

Begtrup, M. *et al.*, *Acta Chem. Scand.*, 1992, **46**, 372, (*oxide*)

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