



>>Entry Name: 4-Methylthiazole, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3716

CAS Registry Number: 693-95-8

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>NS

**Molecular Weight:** 99.156

**Accurate Mass:** 99.014269

**Percentage Composition:** C 48.45%; H 5.08%; N 14.13%; S 32.34%

**Use/Importance:** Flavour ingredient. Present in asparagus, cooked beef, cooked pork, pork liver, coffee, roast barley, roast peanut and cooked shrimp

**Physical Description:** Liq. with nutty, green odour

**Boiling Point:** Bp 130-133°. Bp<sub>59</sub> 70-71°

**Solubility:** Misc. H<sub>2</sub>O

**Density:** d<sub>4</sub><sup>25</sup> 1.11

**pKa Value:** pK<sub>a</sub> 3.15 (25°)

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.5234

Aldrich: W37160-2

>>Derivative: Picrate

**Melting Point:** Mp 181°

>>Derivative: N-Me

**Molecular Formula:** C<sub>5</sub>H<sub>8</sub>NS<sup>(+)</sup>

**Molecular Weight:** 114.191

**Accurate Mass:** 114.037744

**Percentage Composition:** C 52.59%; H 7.06%; N 12.27%; S 28.08%

**Physical Description:** Cryst. (EtOH/Et<sub>2</sub>O) (as iodide)

**Melting Point:** Mp 117-118.5° (iodide)

>>Derivative: N-Et

**Molecular Formula:** C<sub>6</sub>H<sub>10</sub>NS<sup>(+)</sup>

**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/Et<sub>2</sub>O) (as iodide)

**Melting Point:** Mp 169-171° (iodide)

#### References:

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Gisele, D. *et al.*, *Spectrochim. Acta A*, 1967, **23**, 2669, (*ir, Raman*)

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