



>>Entry Name: 4-Methylthiazole, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3716

CAS Registry Number: 693-95-8

Molecular Formula: C₄H₅NS

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°. Bp₅₉ 70-71°

Solubility: Misc. H₂O

Density: d₄²⁵ 1.11

pKa Value: pK_a 3.15 (25°)

Refractive Index: n_D²⁰ 1.5234

Aldrich: W37160-2

>>Derivative: Picrate

Melting Point: Mp 181°

>>Derivative: N-Me

Molecular Formula: C₅H₈NS⁽⁺⁾

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/Et₂O) (as iodide)

Melting Point: Mp 117-118.5° (iodide)

>>Derivative: N-Et

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/Et₂O) (as iodide)

Melting Point: Mp 169-171° (iodide)

References:

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