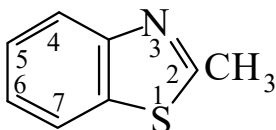




>>Entry Name: 2-Methylbenzothiazole, 9CI

ENTRY UNDER REVIEW



CAS Registry Number: 120-75-2

Related CAS Registry Numbers(s): 14933-76-7

Molecular Formula: C₈H₇NS

Molecular Weight: 149.216

Accurate Mass: 149.029919

Percentage Composition: C 64.40%; H 4.73%; N 9.39%; S 21.49%

Biological Source: Prod. by a *Micrococcus* sp. found in *Tedania ignis*. Also known as an aroma constit. of tea leaves

Melting Point: Mp 14°

Boiling Point: Bp 238°. Bp₁₅ 150-151°

pKa Value: pK_a 2.06 (H₂O) pK_a 8.63 (MeCN)

Hazard & Toxicity: LD₅₀ (mus, ipr) 300 mg/kg

Aldrich: 11214-3

Fluka: 65870

>>Derivative: Picrate

Melting Point: Mp 153.5°

>>Derivative: N-Oxide

CAS Registry Number: 23808-61-9

Molecular Formula: C₈H₇NOS

Molecular Weight: 165.215

Accurate Mass: 165.024834

Percentage Composition: C 58.16%; H 4.27%; N 8.48%; O 9.68%; S 19.41%

Physical Description: Light yellow cryst. + 2H₂O (MeCN aq.)

Melting Point: Mp 46-48°

>>Derivative: N-Et

CAS Registry Number: 3119-93-5

Molecular Formula: C₁₀H₁₂NS⁽⁺⁾

Molecular Weight: 178.278

Accurate Mass: 178.069044

Percentage Composition: C 67.37%; H 6.78%; N 7.86%; S 17.99%

Physical Description: Needles (EtOH)

Melting Point: Mp 196° (as iodide)

Other Data: CAS no. refers to iodide

Aldrich: 37700-7

Fluka: 46102

Rare Chemicals Library: S67193-2

>>Derivative: N-Propyl

CAS Registry Number: 60126-29-6

Molecular Formula: C₁₁H₁₄NS⁽⁺⁾

Molecular Weight: 192.304

Accurate Mass: 192.084694

Percentage Composition: C 68.70%; H 7.34%; N 7.28%; S 16.67%

Use/Importance: Precursor in synth. of carbocyanine dyes

Melting Point: Mp 173-176° (as iodide)

Other Data: CAS no. refers to iodide

Aldrich: 36329-4

Rare Chemicals Library: S65587-2

References: