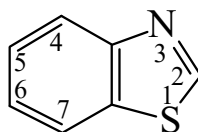




>>Entry Name: Benzothiazole, 9CI



CAS Registry Number: 95-16-9

Molecular Formula: C₇H₅NS

Molecular Weight: 135.189

Accurate Mass: 135.014269

Percentage Composition: C 62.19%; H 3.73%; N 10.36%; S 23.72%

Biological Source: Isol. from tail glands of the red deer *Cervus elaphus* and cranberries

Use/Importance: Used in synth. of α -hydroxy carbonyl compounds

Boiling Point: Bp 223-225°. Bp₂₅ 119-120°

Solubility: Sol. EtOH, CS₂, v. spar. sol. H₂O

pKa Value: pK_a 1.2 (H₂O)

Other Data: Steam-volatile

Hazard & Toxicity: Fl. p. 112°. LD₅₀ (rat, orl) 466 mg/kg; LD₅₀ (mus, orl) 900 mg/kg

Aldrich: W32560-0

Fluka: 12797

>>Derivative: Picrate

Melting Point: Mp 176°

>>Derivative: Methiodide

CAS Registry Number: 2786-31-4

Physical Description: Needles

Melting Point: Mp 210°

Aldrich: 38597-2

>>Derivative: N-Oxide

CAS Registry Number: 27655-38-5

Molecular Formula: C₇H₅NOS

Molecular Weight: 151.189

Accurate Mass: 151.009184

Percentage Composition: C 55.61%; H 3.33%; N 9.26%; O 10.58%; S 21.21%

Physical Description: Prisms + 1H₂O (MeOAc or Et₂O)

Melting Point: Mp 45-48°

>>Derivative: N-Et

see 3-Ethylbenzothiazolium(1+), [MNW49-N](#)

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