



CAS Registry Number: 615-22-5
Molecular Formula: C₈H₇NS₂
Molecular Weight: 181.282
Accurate Mass: 181.001989
Percentage Composition: C 53.00%; H 3.89%; N 7.73%; S 35.38%
Physical Description: Prisms (EtOH aq.)
Melting Point: Mp 52°
Boiling Point: Bp 291-300°. Bp_{0.5} 116°
Aldrich: 16865-3
Rare Chemicals Library: S35301-9

>>Derivative: S-Me; hydroiodide

Physical Description: Cryst. (EtOH)
Melting Point: Mp 128.3°

>>Derivative: S-Me, S,S-dioxide
Synonym(s): 2-(Methylsulfonyl)benzothiazole

CAS Registry Number: 7144-49-2
Molecular Formula: C₈H₇NO₂S₂
Molecular Weight: 213.281
Accurate Mass: 212.991819
Percentage Composition: C 45.05%; H 3.31%; N 6.57%; O 15.00%; S 30.07%
Physical Description: Red solid (EtOH)
Melting Point: Mp 90°

>>Derivative: S-Et
Synonym(s): 2-(Ethylthio)benzothiazole

CAS Registry Number: 2757-92-8
Molecular Formula: C₉H₉NS₂
Molecular Weight: 195.309
Accurate Mass: 195.017639
Percentage Composition: C 55.35%; H 4.64%; N 7.17%; S 32.84%
Physical Description: Cryst. (EtOH)
Boiling Point: Bp₆ 148-150°
Refractive Index: n_D²⁰ 1.6580
Aldrich: 38990-0

>>Derivative: S-Butyl

CAS Registry Number: 2314-17-2
Molecular Formula: C₁₁H₁₃NS₂
Molecular Weight: 223.362
Accurate Mass: 223.048939
Percentage Composition: C 59.15%; H 5.87%; N 6.27%; S 28.71%
Use/Importance: Cotton plant defoliant
Boiling Point: Bp₆ 163-165°

>>Derivative: S-Benzyl
Synonym(s): 2-(Benzylthio)benzothiazole

CAS Registry Number: 19654-17-2
Molecular Formula: C₁₄H₁₁NS₂
Molecular Weight: 257.38
Accurate Mass: 257.033289
Percentage Composition: C 65.33%; H 4.31%; N 5.44%; S 24.92%
Melting Point: Mp 149-150°

>>Derivative: Disulfide
see Di-2-benzothiazolyl disulfide, [BND85-N](#)

References: