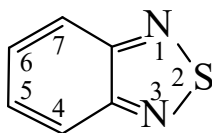




>>Entry Name: **2,1,3-Benzothiadiazole**, 9CI

Synonym(s): 2-Thia-1,3-diaza-2*H*-isoindene. 1,3-Dihydro-2,1,3-benzothiadiazole. Benzisothiadiazole. **Piazthiole (obsol.)**‡



CAS Registry Number: 273-13-2

Molecular Formula: C₆H₄N₂S

Molecular Weight: 136.177

Accurate Mass: 136.009518

Percentage Composition: C 52.92%; H 2.96%; N 20.57%; S 23.55%

Physical Description: Needles with quinoxaline-like odour

Melting Point: Mp 44°

Boiling Point: Bp 206°

Solubility: Spar. sol. H₂O

Other Data: Steam-volatile. Zn + HCl → *o*-Phenylenediamine

Aldrich: B1090-0

Fluka: 12794

>>Derivative: *N*¹-Oxide

CAS Registry Number: 23431-06-3

Molecular Formula: C₆H₄N₂OS

Molecular Weight: 152.176

Accurate Mass: 152.004433

Percentage Composition: C 47.36%; H 2.65%; N 18.41%; O 10.51%; S 21.07%

Physical Description: Yellow cryst.

Melting Point: Mp 78-80°

>>Derivative: *S*-Oxide

CAS Registry Number: 69201-99-6

Molecular Formula: C₆H₄N₂OS

Molecular Weight: 152.176

Accurate Mass: 152.004433

Percentage Composition: C 47.36%; H 2.65%; N 18.41%; O 10.51%; S 21.07%

Physical Description: Yellow cryst. (MeOH)

Melting Point: Mp 86-87°

>>Derivative: *S,S*-Dioxide

CAS Registry Number: 1615-06-1

Molecular Formula: C₆H₄N₂O₂S

Molecular Weight: 168.176

Accurate Mass: 167.999348

Percentage Composition: C 42.85%; H 2.40%; N 16.66%; O 19.03%; S 19.07%

Melting Point: Mp 178-180°

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