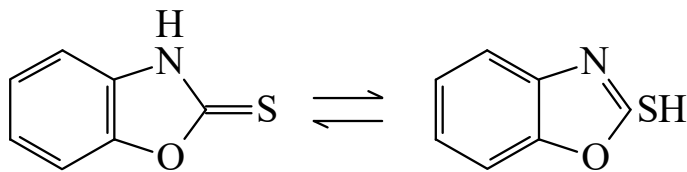




>>Entry Name: **2(3*H*)-Benzoxazolethione, 9Cl**

Synonym(s): 2-Benzoxazolinethione, 8Cl. 2-Benzoxazolethiol, 8Cl. 2-Mercaptobenzoxazole



CAS Registry Number: 2382-96-9

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%

Use/Importance: Reagent for prepn. of sulfides. Used as 0.15% soln. in aq. dioxan for photometric detn. of Os, Pd

Physical Description: Needles (H₂O)

Melting Point: Mp 196°

Solubility: Spar. sol. H₂O, EtOH

pK_a Value: pK_a 6.33 (25°)

Other Data: HCl at 170° → CO₂ + H₂S + 2-Aminophenol

Aldrich: M350-7

Fluka: 63750

>>Variant: *NH*-form

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%

>>Derivative: 3-Ac

CAS Registry Number: 37441-95-5

Molecular Formula: C₉H₇NO₂S

Molecular Weight: 193.226

Accurate Mass: 193.019749

Percentage Composition: C 55.94%; H 3.65%; N 7.25%; O 16.56%; S 16.60%

Physical Description: Plates

Melting Point: Mp 117°

>>Derivative: 3-Me

CAS Registry Number: 13673-63-7

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: Needles (EtOH)

Melting Point: Mp 132°

>>Derivative: 3-Et

CAS Registry Number: 40888-01-5

Molecular Formula: C₉H₉NOS

Molecular Weight: 179.242

Accurate Mass: 179.040484

Percentage Composition: C 60.31%; H 5.06%; N 7.81%; O 8.93%; S 17.89%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 112°