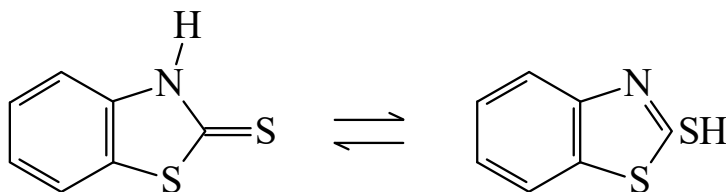




>>Entry Name: **2(3*H*)-Benzothiazolethione**, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Benzothiazolethiol. 2-Mercaptobenzothiazole. 2-Benzothiazolinethione. Accelerator M. Accel M. Pneumax MBT. Thiotax



CAS Registry Number: 149-30-4

Related CAS Registry Numbers(s): 155-04-4 2492-26-4 37437-20-0

Molecular Formula: C₇H₅NS₂

Molecular Weight: 167.255

Accurate Mass: 166.986339

Percentage Composition: C 50.27%; H 3.01%; N 8.37%; S 38.34%

General Statement: *NH*-form predominates

Biological Source: Isol. from a *Micrococcus* sp. in *Tedania ignis*

Use/Importance: Vulcanisation accelerator. Used as 1% CHCl₃ soln. for separation pptn. of Au, I⁽⁻⁾; photometric detn. of Pd, Os, Rh, Se, Ni ($\lambda_{\max}$ 750 nm)

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 177-179°

Solubility: Spar. sol. EtOH, Et₂O, AcOH; insol. H₂O; sol. alkalis

Other Data: Readily oxidised to the disulfide

Hazard & Toxicity: LD₅₀ (rat, orl) 100 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects

Aldrich: M330-2

Fluka: 63730

Sigma: M2274

>>Variant: *NH*-form

Molecular Formula: C₇H₅NS₂

Molecular Weight: 167.255

Accurate Mass: 166.986339

Percentage Composition: C 50.27%; H 3.01%; N 8.37%; S 38.34%

>>Derivative: *N*-Me

CAS Registry Number: 2254-94-6

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%

Use/Importance: Reagent for stereospecific prepn. of thiirans from oxiranes

Physical Description: Cryst. (petrol)

Melting Point: Mp 92° (89-90°)

Boiling Point: Bp_{0.5} 156°

Aldrich: M3000-0

>>Derivative: *N*-Et

CAS Registry Number: 16407-34-4

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%

Melting Point: Mp 73-75°

>>Variant: *SH*-form

Molecular Formula: C₇H₅NS₂

Molecular Weight: 167.255

Accurate Mass: 166.986339

Percentage Composition: C 50.27%; H 3.01%; N 8.37%; S 38.34%