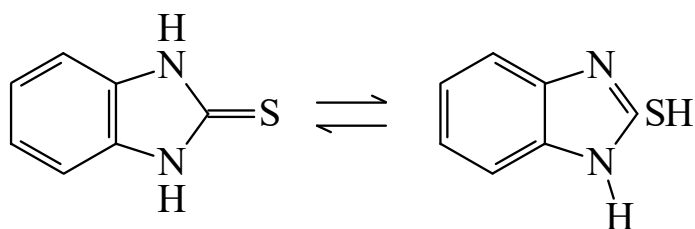




>>Entry Name: **2(1*H*)-Benzimidazolinethione**, 8Cl

Synonym(s): 1,3-Dihydro-2*H*-benzimidazole-2-thione, 9Cl. 1*H*-Benzimidazole-2-thiol. 2-Benzimidazolethiol. 2-Mercaptobenzimidazole



CAS Registry Number: 583-39-1

Related CAS Registry Numbers(s): 3030-80-6

Molecular Formula: C₇H₆N₂S

Molecular Weight: 150.204

Accurate Mass: 150.025168

Percentage Composition: C 55.98%; H 4.03%; N 18.65%; S 21.35%

General Statement: Thione form predominates

Use/Importance: Antioxidant for polymers, corrosion inhibitor. Used as 1% EtOH soln. for photometric detn. of Se (λ_{max} 325 nm, ϵ 10500); gravimetric detn. of Bi, Cu, Cd, Pb, Hg, Au

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 298° (292-293°)

Solubility: Sol. EtOH; spar. sol. H₂O

pKa Value: p*K*_{a1} 9.18; p*K*_{a2} 10.98 (20°)

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 476 mg/kg

Aldrich: M320-5

Fluka: 63710

>>Derivative: *N*¹-Me

CAS Registry Number: 2360-22-7

Molecular Formula: C₈H₈N₂S

Molecular Weight: 164.231

Accurate Mass: 164.040818

Percentage Composition: C 58.51%; H 4.91%; N 17.06%; S 19.52%

Melting Point: Mp 190-192°

>>Derivative: *N*¹-Ph

CAS Registry Number: 4493-32-7

Molecular Formula: C₁₃H₁₀N₂S

Molecular Weight: 226.301

Accurate Mass: 226.056468

Percentage Composition: C 69.00%; H 4.45%; N 12.38%; S 14.17%

Melting Point: Mp 194-195°

Rare Chemicals Library: S7084-0

>>Derivative: *N*¹-Benzyl

CAS Registry Number: 31493-51-3

Molecular Formula: C₁₄H₁₂N₂S

Molecular Weight: 240.328

Accurate Mass: 240.072118

Percentage Composition: C 69.97%; H 5.03%; N 11.66%; S 13.34%

Melting Point: Mp 181-182°

>>Variant: Thione-form

Molecular Formula: C₇H₆N₂S

Molecular Weight: 150.204

Accurate Mass: 150.025168

Percentage Composition: C 55.98%; H 4.03%; N 18.65%; S 21.35%