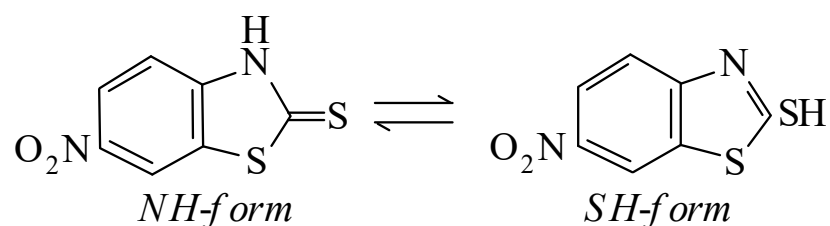




>>Entry Name: 6-Nitro-2(3*H*)-benzothiazolethione, 9Cl

Synonym(s): 6-Nitro-2-benzothiazolethiol. 2-Mercapto-6-nitrobenzothiazole



CAS Registry Number: 4845-58-3

Molecular Formula: C₇H₄N₂O₂S₂

Molecular Weight: 212.253

Accurate Mass: 211.971418

Percentage Composition: C 39.61%; H 1.90%; N 13.20%; O 15.08%; S 30.21%

Use/Importance: Reagent for the identification of alkyl halides

Physical Description: Yellow needles (AcOH)

Melting Point: Mp 255-257°

Hazard & Toxicity: LD₅₀ (mus, ipr) 25 mg/kg

>>Variant: *SH*-form

Molecular Formula: C₇H₄N₂O₂S₂

Molecular Weight: 212.253

Accurate Mass: 211.971418

Percentage Composition: C 39.61%; H 1.90%; N 13.20%; O 15.08%; S 30.21%

>>Derivative: S-Me

Synonym(s): 2-(Methylthio)-6-nitrobenzothiazole

CAS Registry Number: 3621-99-6

Molecular Formula: C₈H₆N₂O₂S₂

Molecular Weight: 226.28

Accurate Mass: 225.987068

Percentage Composition: C 42.46%; H 2.67%; N 12.38%; O 14.14%; S 28.34%

Physical Description: Pale-yellow needles

Melting Point: Mp 128°

>>Derivative: S-Et

Synonym(s): 2-(Ethylthio)-6-nitrobenzothiazole

CAS Registry Number: 65611-80-5

Molecular Formula: C₉H₈N₂O₂S₂

Molecular Weight: 240.306

Accurate Mass: 240.002718

Percentage Composition: C 44.98%; H 3.36%; N 11.66%; O 13.32%; S 26.69%

Physical Description: Pale-yellow needles

Melting Point: Mp 106-108°

>>Derivative: Disulfide

Molecular Formula: C₁₄H₆N₄O₄S₄

Molecular Weight: 422.49

Accurate Mass: 421.927186

Percentage Composition: C 39.80%; H 1.43%; N 13.26%; O 15.15%; S 30.36%

Physical Description: Pale-yellow needles

Melting Point: Mp 229-231°

References:

Sebrell, L.B. *et al.*, *J.A.C.S.*, 1927, **49**, 1780, (*synth*)

Fr. Pat., 1933, 741 910; *CA*, **27**, 3642

Takahashi, T. *et al.*, *Yakugaku Zasshi*, 1946, **66**, 24; *CA*, **45**, 8532

Cutter, H.B. *et al.*, *J.A.C.S.*, 1947, **69**, 831, (*use*)

Faure, R. *et al.*, *Org. Magn. Reson.*, 1978, **11**, 617, (*cmr, tautom*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MCP250