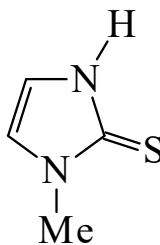




>>Entry Name: 1,3-Dihydro-1-methyl-2*H*-imidazole-2-thione, 9CI

Synonym(s): 1-Methyl-2-imidazolethiol, 8CI. 2-Mercapto-1-methylimidazole. Methimazole, BAN. **Thiamazole**, INN. Mercazolyl. Metimazol. Tapazole. Many other names



CAS Registry Number: 60-56-0

Related CAS Registry Numbers(s): 119393-94-1 135011-47-1

Molecular Formula: C₄H₆N₂S

Molecular Weight: 114.171

Accurate Mass: 114.025168

Percentage Composition: C 42.08%; H 5.30%; N 24.54%; S 28.09%

Use/Importance: Used in treatment of hyperthyroidism

Physical Description: Leaflets (EtOH)

Melting Point: Mp 146-148°

Boiling Point: Bp 280° dec.

Calculated Log P Data: Log P -0.34 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 2250 mg/kg. Human and exp. teratogenic effects. Exp. neoplastigenic data and reprod. effects

Aldrich: 30150-7

Fluka: 63760

Sigma: M8506

>>Derivative: 3-Ac

CAS Registry Number: 15033-52-0

Molecular Formula: C₆H₈N₂OS

Molecular Weight: 156.208

Accurate Mass: 156.035733

Percentage Composition: C 46.13%; H 5.16%; N 17.93%; O 10.24%; S 20.53%

Physical Description: Needles

Melting Point: Mp 72-74°

>>Derivative: 3-Benzoyl

CAS Registry Number: 15033-66-6

Molecular Formula: C₁₁H₁₀N₂OS

Molecular Weight: 218.279

Accurate Mass: 218.051383

Percentage Composition: C 60.53%; H 4.62%; N 12.83%; O 7.33%; S 14.69%

Physical Description: Yellow needles

Melting Point: Mp 98-100°

>>Derivative: 3-Me

see 1,3-Dihydro-1,3-dimethyl-2*H*-imidazole-2-thione, [CZW50-H](#)

>>Derivative: 3-Et

Synonym(s): 1-Ethyl-1,3-dihydro-3-methyl-2*H*-imidazole-2-thione

CAS Registry Number: 61640-28-6

Molecular Formula: C₆H₁₀N₂S

Molecular Weight: 142.224

Accurate Mass: 142.056468

Percentage Composition: C 50.67%; H 7.09%; N 19.70%; S 22.55%

Melting Point: Mp 51°