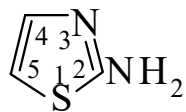




>>Entry Name: 2-Aminothiazole

Synonym(s): 2-Thiazolamine, 9Cl. **Aminothiazole**, INN. Abadol. RP 2921



CAS Registry Number: 96-50-4

Related CAS Registry Numbers(s): 61169-63-9

Molecular Formula: C₃H₄N₂S

Molecular Weight: 100.144

Accurate Mass: 100.009518

Percentage Composition: C 35.98%; H 4.03%; N 27.97%; S 32.02%

Use/Importance: Thyroid inhibitor; metal corrosion inhibitor

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 90°

Boiling Point: Bp₁₁ 140°

pKa Value: pK_a 5.32 (25°)

Calculated Log P Data: Log P 0.22 (calc)

Hazard & Toxicity: Ignited in drying oven. Violent explosion when nitrated with nitric/sulfuric acids. LD₅₀ (rat, orl) 480 mg/kg

Aldrich: 12312-9

Fluka: 9480

Sigma: A0147

>>Derivative: *N*-Ac

CAS Registry Number: 2719-23-5

Molecular Formula: C₅H₆N₂OS

Molecular Weight: 142.181

Accurate Mass: 142.020083

Percentage Composition: C 42.24%; H 4.25%; N 19.70%; O 11.25%; S 22.55%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 203°

Rare Chemicals Library: S41396-8

>>Derivative: *N*-Benzoyl

CAS Registry Number: 13053-82-2

Molecular Formula: C₁₀H₈N₂OS

Molecular Weight: 204.252

Accurate Mass: 204.035733

Percentage Composition: C 58.80%; H 3.95%; N 13.72%; O 7.83%; S 15.70%

Melting Point: Mp 152°

>>Derivative: *N*-Me

CAS Registry Number: 6142-06-9

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%

Melting Point: Mp 80-82°

>>Derivative: *N*-Et

CAS Registry Number: 13472-75-8

Molecular Formula: C₅H₈N₂S

Molecular Weight: 128.198

Accurate Mass: 128.040818

Percentage Composition: C 46.85%; H 6.29%; N 21.85%; S 25.01%

Melting Point: Mp 49-50°