



>>Entry Name: 3-Amino-4-pyridinethiol

Synonym(s): 3-Amino-4(1*H*)-pyridinethione, 9Cl. 3-Amino-4-mercaptopyridine

CAS Registry Number: 89002-13-1

Related CAS Registry Numbers(s): 38240-23-2 59243-59-3 59243-62-8

Molecular Formula: C₅H₆N₂S

Molecular Weight: 126.182

Accurate Mass: 126.025168

Percentage Composition: C 47.59%; H 4.79%; N 22.20%; S 25.41%

General Statement: Thione form likely to predominate

Use/Importance: Intermed. for cephalosporins

Physical Description: Pale yellow granules (H₂O)

Melting Point: Mp 213 dec.°

Solubility: Sol. aq. alkalies

>>Derivative: *N*-Ac, *S*-Me

Molecular Formula: C₈H₁₀N₂OS

Molecular Weight: 182.246

Accurate Mass: 182.051383

Percentage Composition: C 52.72%; H 5.53%; N 15.37%; O 8.78%; S 17.59%

Physical Description: Granules +½H₂O (Me₂CO)

Melting Point: Mp 109 approx.°

>>Derivative: *S*-Me

Synonym(s): 4-(Methylthio)-3-pyridinamine. 3-Amino-4-methylthiopyridine

CAS Registry Number: 38240-24-3

Molecular Formula: C₆H₈N₂S

Molecular Weight: 140.209

Accurate Mass: 140.040818

Percentage Composition: C 51.40%; H 5.75%; N 19.98%; S 22.87%

Physical Description: Yellow needles (MeOH) (as picrate)

Melting Point: Mp 173-174° (165-166°) (picrate)

>>Derivative: *S*-Et

Synonym(s): 4-(Ethylthio)-3-pyridinamine. 3-Amino-4-ethylthiopyridine

Molecular Formula: C₇H₁₀N₂S

Molecular Weight: 154.235

Accurate Mass: 154.056468

Percentage Composition: C 54.51%; H 6.53%; N 18.16%; S 20.79%

Physical Description: Needles (EtOH) (as hydrochloride)

Melting Point: Mp 213 dec.° (hydrochloride)

References:

Takahashi, T. *et al.*, *Chem. Pharm. Bull.*, 1954, **2**, 196; 1955, **3**, 356, (*synth, derivs*)

Barlin, G.B., *J.C.S. Perkin 2*, 1972, 1459, (*synth, uv, props*)