



Use/Importance: Used as 0.5% aq. soln. for detn. of $\text{I}^{(-)}$, $\text{IO}_3^{(-)}$, Bi(III)

Physical Description: Cryst.

Melting Point: Mp 67-69°

Solubility: Sol. EtOH, CHCl_3 ; sl. sol. H_2O

>> **Derivative:** 1-Acetic acid

CAS Registry Number: 57658-36-3

Molecular Formula: $\text{C}_3\text{H}_4\text{N}_4\text{O}_2\text{S}$

Molecular Weight: 160.156

Accurate Mass: 160.005496

Percentage Composition: C 22.50%; H 2.52%; N 34.98%; O 19.98%; S 20.02%

Melting Point: Mp 179-180°

>> **Variant:** 1,4-Dihydro-form

Molecular Formula: $\text{CH}_2\text{N}_4\text{S}$

Molecular Weight: 102.12

Accurate Mass: 102.000016

Percentage Composition: C 11.76%; H 1.97%; N 54.86%; S 31.40%

>> **Derivative:** 1,4-Di-Me

CAS Registry Number: 54986-14-0

Molecular Formula: $\text{C}_3\text{H}_6\text{N}_4\text{S}$

Molecular Weight: 130.173

Accurate Mass: 130.031316

Percentage Composition: C 27.68%; H 4.65%; N 43.04%; S 24.63%

Physical Description: Cryst. (petrol)

Melting Point: Mp 99-100°. Mp 107°

>> **Derivative:** 1-Me, 4-Ph

CAS Registry Number: 1455-91-0

Molecular Formula: $\text{C}_8\text{H}_8\text{N}_4\text{S}$

Molecular Weight: 192.244

Accurate Mass: 192.046966

Percentage Composition: C 49.98%; H 4.19%; N 29.14%; S 16.68%

Physical Description: Cryst.

Melting Point: Mp 47-49°

>> **Variant:** 1,3-Dihydro-form

Molecular Formula: $\text{CH}_2\text{N}_4\text{S}$

Molecular Weight: 102.12

Accurate Mass: 102.000016

Percentage Composition: C 11.76%; H 1.97%; N 54.86%; S 31.40%

>> **Derivative:** 3-Et, 1-Ph

CAS Registry Number: 62681-14-5

Molecular Formula: $\text{C}_9\text{H}_{10}\text{N}_4\text{S}$

Molecular Weight: 206.271

Accurate Mass: 206.062616

Percentage Composition: C 52.41%; H 4.89%; N 27.16%; S 15.55%

Physical Description: Yellowish-white prisms (EtOAc/hexane)

Melting Point: Mp 114.5-115°

>> **Variant:** *SH*-form

CAS Registry Number: 18686-81-2

Molecular Formula: $\text{CH}_2\text{N}_4\text{S}$

Molecular Weight: 102.12

Accurate Mass: 102.000016

Percentage Composition: C 11.76%; H 1.97%; N 54.86%; S 31.40%

Rare Chemicals Library: S14331-6