



>>Entry Name: Thiourea, 9CI

ENTRY UNDER REVIEW

Synonym(s): Thiocarbamide. Thiocarbonic diamide

CAS Registry Number: 62-56-6

H_2NCSNH_2

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

Molecular Weight: 76.122

Accurate Mass: 76.009518

Percentage Composition: C 15.78%; H 5.30%; N 36.80%; S 42.12%

Use/Importance: Photographic fixer. Forms separable inclusion complexes. Used in heterocyclic synth. Used as 10% aq. soln. for photometric detn. of Bi (λ_{max} 470 nm, ϵ 9000), Os, Ru, Re, Se, Te; reducing agent

Physical Description: Rhombohedra or needles (EtOH)

Melting Point: Mp 175-177°. Mp 180°

Solubility: Sol. H_2O , EtOH; spar. sol. Et_2O

pKa Value: $\text{p}K_{\text{a}} -1.19$ (20°, H_2SO_4 aq.)

Hazard & Toxicity: Possible human carcinogen. Adverse haemopoietic effects reported by ingestion. LD_{50} (rat, orl) 125 mg/kg. Exp. carcinogen and teratogen. Exp. reprod. effects. Hepatotoxic

Aldrich: 24025-7

Fluka: 88810

Sigma: T8656

>>Derivative: Hydrochloride

Melting Point: Mp 136-137°

>>Derivative: *N*-Ac

Synonym(s): *N*-(Aminothioxomethyl)acetamide, 9CI. 1-Acetyl-2-thiourea, 8CI

CAS Registry Number: 591-08-2

Use/Importance: Reagent for synth. of thiols

Physical Description: Needles

Melting Point: Mp 165°

Hazard & Toxicity: LD_{50} (rat, orl) 50 mg/kg

Aldrich: A2285-8

Fluka: 1485

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

Molecular Formula: $\text{C}_5\text{H}_8\text{N}_2\text{O}_2\text{S}$

Molecular Weight: 160.196

Accurate Mass: 160.030648

Percentage Composition: C 37.49%; H 5.03%; N 17.49%; O 19.97%; S 20.02%

Physical Description: Yellow prisms (AcOH aq.)

Melting Point: Mp 153°

>>Derivative: *N*-Benzoyl

>>Derivative: *N*-Me

>>Derivative: *N,N*-Di-Me

>>Derivative: *N,N'*-Di-Me