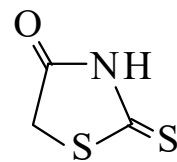




>>Entry Name: 2-Thioxo-4-thiazolidinone, 9CI
Synonym(s): Rhodanine. Rhodanic acid. Rhodamine



CAS Registry Number: 141-84-4

Molecular Formula: C₃H₃NOS₂
Molecular Weight: 133.195
Accurate Mass: 132.965604
Percentage Composition: C 27.05%; H 2.27%; N 10.52%; O 12.01%; S 48.15%

Use/Importance: Intermed. in Phenylalanine synth. Reagent for the photometric detn. of gallic acid

Physical Description: Pale yellow prisms (EtOH)

Melting Point: Mp 170°

pKa Value: p*K*_{a1} 5.18 (20°, 0.1*M* NaClO₄)

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 326 mg/kg

Aldrich: 11819-2

Fluka: 83700

Sigma: R4375

>>Derivative: *N*-Me

Synonym(s): 3-Methylrhodanine

CAS Registry Number: 4807-55-0

Molecular Formula: C₄H₅NOS₂

Molecular Weight: 147.222

Accurate Mass: 146.981254

Percentage Composition: C 32.63%; H 3.42%; N 9.51%; O 10.87%; S 43.56%

Use/Importance: Shows antispasmodic activity

Melting Point: Mp 69-71°

Aldrich: M8045-8

Rare Chemicals Library: S42819-1

>>Derivative: *N*-Et

Synonym(s): 3-Ethyl-2-thioxo-4-thiazolidinone, 9CI. 3-Ethylrhodanine

CAS Registry Number: 7648-01-3

Molecular Formula: C₅H₇NOS₂

Molecular Weight: 161.248

Accurate Mass: 160.996904

Percentage Composition: C 37.24%; H 4.38%; N 8.69%; O 9.92%; S 39.77%

Use/Importance: Reagent for the spectrophotometric anal. of *p*-quinones

Melting Point: Mp 36-36.5°

Aldrich: 38577-8

Rare Chemicals Library: S53351-3

>>Derivative: *N*-(2-Propenyl)

CAS Registry Number: 1457-47-2

Molecular Formula: C₆H₇NOS₂

Molecular Weight: 173.259

Accurate Mass: 172.996904

Percentage Composition: C 41.59%; H 4.07%; N 8.08%; O 9.23%; S 37.02%

Melting Point: Mp 46-48°

Boiling Point: Bp₆ 139°

Aldrich: A3560-7

Rare Chemicals Library: S28164-6