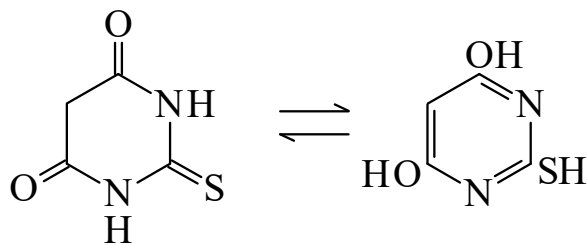




>>>Entry Name: Dihydro-2-thioxo-4,6-(1*H*,5*H*)-pyrimidinedione, 9CI

Synonym(s): 4,6-Dihydroxy-2-mercaptopyrimidine. 2-Mercapto-4,6-pyrimidinediol. Thiobarbituric acid. Malonylthiourea. Bathyran. Monothiobarbituric acid. Austranal



CAS Registry Number: 504-17-6

Related CAS Registry Numbers(s): 31645-12-2

Molecular Formula: C₄H₄N₂O₂S

Molecular Weight: 144.154

Accurate Mass: 143.999348

Percentage Composition: C 33.33%; H 2.80%; N 19.43%; O 22.20%; S 22.24%

General Statement: Di-*NH* (thioxo) tautomer predominates. Intermediate tautomers also possible

Use/Importance: Bactericide, thyroid inhibitor. Used as 0.03*M* aq. soln. for photometric detn. of Bi, Cu, Pd, Ru(*III*) (λ_{max} 338 nm, ϵ 11000)

Physical Description: Plates (H₂O)

Melting Point: Mp 235 dec.° (rapid heating)

Solubility: Sol. H₂O, alkalis

Hazard & Toxicity: LD₅₀ (mus, ipr) 600 mg/kg

Aldrich: D11350-6

Fluka: 88481

Sigma: T1156

>>>Variant: Di-*NH*-form

Molecular Formula: C₄H₄N₂O₂S

Molecular Weight: 144.154

Accurate Mass: 143.999348

Percentage Composition: C 33.33%; H 2.80%; N 19.43%; O 22.20%; S 22.24%

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

Synonym(s): 1,3-Diethyl-2-thiobarbituric acid

CAS Registry Number: 5217-47-0

Molecular Formula: C₈H₁₂N₂O₂S

Molecular Weight: 200.261

Accurate Mass: 200.061948

Percentage Composition: C 47.98%; H 6.04%; N 13.99%; O 15.98%; S 16.01%

Melting Point: Mp 109-112°

Aldrich: 16195-0

Sigma: D6257

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

Synonym(s): 1,3-Diphenyl-2-thiobarbituric acid. Dihydro-1,3-diphenyl-2-thioxo-4,6-(1*H*,5*H*)-pyrimidinedione, 9CI

CAS Registry Number: 35221-12-6

Molecular Formula: C₁₆H₁₂N₂O₂S

Molecular Weight: 296.349

Accurate Mass: 296.061948

Percentage Composition: C 64.85%; H 4.08%; N 9.45%; O 10.80%; S 10.82%

Use/Importance: Fluorescence labelling reagent used in hplc anal. of lipoperoxides

Physical Description: Cryst. (EtOH)

Melting Point: Mp 216 , 245°°

Aldrich: 46576-3

>>>Variant: Diol-form

Molecular Formula: C₄H₄N₂O₂S

Molecular Weight: 144.154

Accurate Mass: 143.999348

Percentage Composition: C 33.33%; H 2.80%; N 19.43%; O 22.20%; S 22.24%