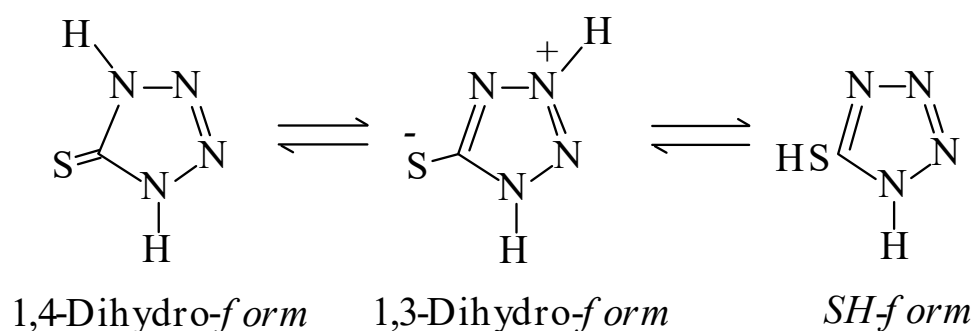




>>Entry Name: 1,4-Dihydro-5*H*-tetrazole-5-thione, 9CI

Synonym(s): Tetrazole-5-thione. 1*H*-Tetrazole-5-thiol. 5-Mercapto-1*H*-tetrazole



Related CAS Registry Numbers(s): 1437-66-7 51138-06-8

Molecular Formula: CH₂N₄S

Molecular Weight: 102.12

Accurate Mass: 102.000016

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

General Statement: 1,4-Dihydro form predominates

Physical Description: Needles

Melting Point: Mp 205 dec.°

>>Derivative: 1-Me

Synonym(s): 1,2-Dihydro-1-methyl-5*H*-tetrazole-5-thione, 9CI. 1-Methyl-1*H*-tetrazole-5-thiol, 8CI. 1-Methyltetrazoline-5-thione

CAS Registry Number: 13183-79-4

Molecular Formula: C₂H₄N₄S

Molecular Weight: 116.146

Accurate Mass: 116.015666

Percentage Composition: C 20.68%; H 3.47%; N 48.24%; S 27.61%

Use/Importance: Metab. of antibiotics containing *N*-methylthiotetrazole side-chain such as Latamoxef [DMF30-S](#)

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 125-126° (121-122°)

pKa Value: p*K*_a 3.86 (50% EtOH aq.)

Other Data: Exists almost entirely in thione form

Aldrich: 35787-1

>>Derivative: 1-Et

Molecular Formula: C₃H₆N₄S

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. (Me₂CO)

Melting Point: Mp 50°

>>Derivative: 1-Ph

CAS Registry Number: 86-93-1

Molecular Formula: C₇H₆N₄S

Molecular Weight: 178.217

Accurate Mass: 178.031316

Percentage Composition: C 47.18%; H 3.39%; N 31.44%; S 17.99%

Use/Importance: Used as 0.05% CHCl₃ soln. for extraction-photometric detn. of Pd ($\lambda_{\max}$ 400 nm, ϵ 2600), Pt. Used as a 2% soln. in EtOH or Me₂CO for detn. of Bi

Physical Description: Faint-yellow cryst. (EtOH)

Melting Point: Mp 151-153° (150°)

Solubility: Sol. CHCl₃, AcOH, EtOH

pKa Value: p*K*_{a1} 2.8 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 250 mg/kg

Aldrich: 16989-7

Fluka: 78820

Rare Chemicals Library: S26960-3

Sigma: P3316