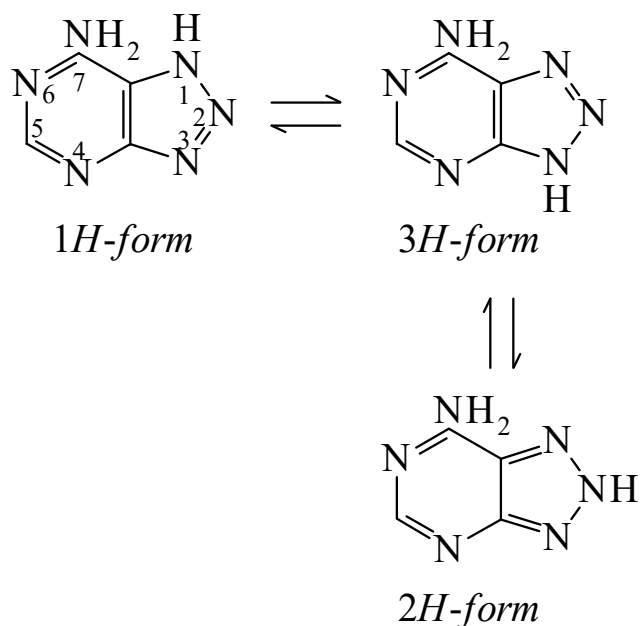




>>Entry Name: 7-Amino-1*H*-1,2,3-triazolo[4,5-*d*]pyrimidine

Synonym(s): 1*H*-1,2,3-Triazolo[4,5-*d*]pyrimidin-7-amine, 9Cl. 8-Azaadenine



CAS Registry Number: 1123-54-2

Molecular Formula: C₄H₄N₆

Molecular Weight: 136.116

Accurate Mass: 136.049744

Percentage Composition: C 35.30%; H 2.96%; N 61.74%

Use/Importance: Purine antagonist

Physical Description: Cryst. (H₂O)

Melting Point: Mp 310 dec., 345° dec.°

Aldrich: 85552-9

Fluka: 11370

Sigma: A5883

>>Variant: 1*H*-form

Molecular Formula: C₄H₄N₆

Molecular Weight: 136.116

Accurate Mass: 136.049744

Percentage Composition: C 35.30%; H 2.96%; N 61.74%

>>Derivative: 1-Me

Molecular Formula: C₅H₆N₆

Molecular Weight: 150.143

Accurate Mass: 150.065394

Percentage Composition: C 40.00%; H 4.03%; N 55.97%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 300°

>>Variant: 3*H*-form

Molecular Formula: C₄H₄N₆

Molecular Weight: 136.116

Accurate Mass: 136.049744

Percentage Composition: C 35.30%; H 2.96%; N 61.74%

>>Derivative: 3-Me

Molecular Formula: C₅H₆N₆

Molecular Weight: 150.143

Accurate Mass: 150.065394

Percentage Composition: C 40.00%; H 4.03%; N 55.97%

Physical Description: Sl. yellow needles (MeOH)

Melting Point: Mp 314-315°