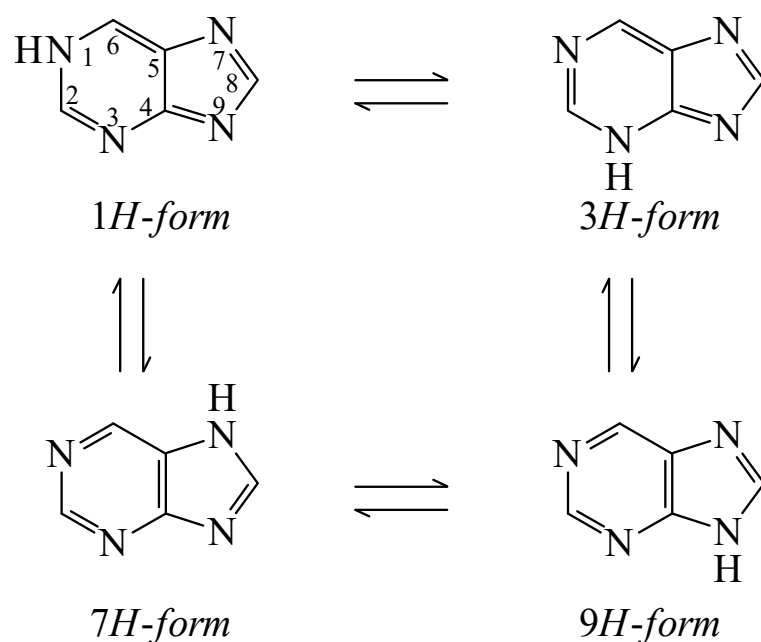




>>Entry Name: Purine

Synonym(s): 3*H*-Imidazo[4,5-*d*]pyrimidine. 3,5,7-Triazaindole



CAS Registry Number: 120-73-0

Molecular Formula: C₅H₄N₄

Molecular Weight: 120.113

Accurate Mass: 120.043596

Percentage Composition: C 50.00%; H 3.36%; N 46.64%

Physical Description: Needles (EtOH or toluene)

Melting Point: Mp 216-217°

pKa Value: p*K*_{a1} 2.3; p*K*_{a2} 8.96 (20°)

Aldrich: P5580-5

Fluka: 82580

Sigma: P1655

>>Derivative: Hydrochloride

Physical Description: Cryst. (H₂O)

Melting Point: Mp 206-207°

>>Derivative: Nitrate

Physical Description: Cryst. (H₂O)

Melting Point: Mp 205 dec.°

>>Derivative: 3*N*-Oxide

CAS Registry Number: 67900-85-0

Molecular Formula: C₅H₄N₄O

Molecular Weight: 136.113

Accurate Mass: 136.038511

Percentage Composition: C 44.12%; H 2.96%; N 41.16%; O 11.75%

Hazard & Toxicity: Exp. carcinogen

>>Variant: 1*H*-form

Molecular Formula: C₅H₄N₄

Molecular Weight: 120.113

Accurate Mass: 120.043596

Percentage Composition: C 50.00%; H 3.36%; N 46.64%