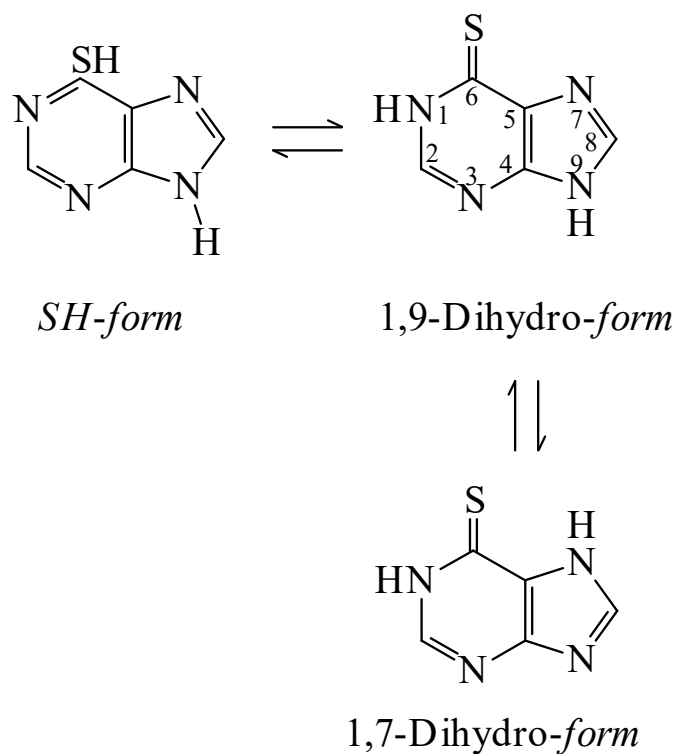




>>Entry Name: 6-Purinethiol

Synonym(s): 1,7-Dihydro-6*H*-purine-6-thione, 9Cl. 6-Mercaptopurine. **Mercaptopurine**, BAN, INN, USAN. Thiohypoxanthine. Ismipur. Leukerin. NSC 755. WR 2785



CAS Registry Number: 50-44-2

Related CAS Registry Numbers(s): 6112-76-1

Molecular Formula: C₅H₄N₄S

Molecular Weight: 152.179

Accurate Mass: 152.015666

Percentage Composition: C 39.46%; H 2.65%; N 36.82%; S 21.07%

Use/Importance: Inhibitor of purine metabolism; antineoplastic agent (for acute leukaemia)

Physical Description: Yellow prisms + 1H₂O (H₂O)

Melting Point: Mp 313-314 dec.° (loses H₂O at 140°)

pKa Value: p*K*_{a1} 7.77; p*K*_{a2} 10.84 (20°)

Hazard & Toxicity: Systemic effects in humans when used therapeutically. Exp. reprod. and teratogenic effects. LD₅₀ (mus, orl) 260 mg/kg

Rare Chemicals Library: S1437-1

>>Derivative: 7-Oxide

CAS Registry Number: 157871-31-3

Molecular Formula: C₅H₄N₄OS

Molecular Weight: 168.179

Accurate Mass: 168.010581

Percentage Composition: C 35.71%; H 2.40%; N 33.31%; O 9.51%; S 19.07%

Physical Description: Yellow needles

Melting Point: Mp 300 dec.°

pKa Value: p*K*_{a2} 4.9; p*K*_{a3} 9.17 (30°, H₂O)

Other Data: Exists predominantly as 7-hydroxy tautomer in neutral soln.

>>Variant: SH-form

Molecular Formula: C₅H₄N₄S

Molecular Weight: 152.179

Accurate Mass: 152.015666

Percentage Composition: C 39.46%; H 2.65%; N 36.82%; S 21.07%