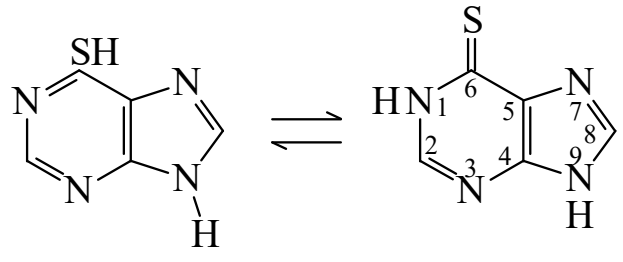
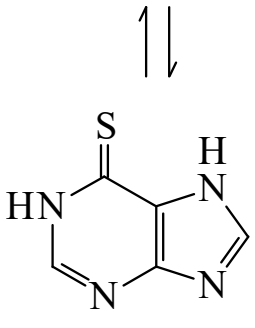
>>**Entry Name: 6-Purinethiol**

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



SH-form 1,9-Dihydro-*form*



1,7-Dihydro-*form*

CAS Registry Number: 50-44-2
Related CAS Registry Numbers(s): 6112-76-1

Molecular Formula: $C_5H_4N_4S$
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 + $1H_2O$ (H_2O)
Melting Point: Mp 313-314 dec.° (loses H_2O at 140°)
pKa Value: pK_{a1} 7.77; pK_{a2} 10.84 (20°)
Hazard & Toxicity: Systemic effects in humans when used therapeutically. Exp. reprod. and teratogenic effects. LD_{50} (mus, orl) 260 mg/kg

Rare Chemicals Library: S1437-1

>>**Derivative:** 7-Oxide

CAS Registry Number: 157871-31-3
Molecular Formula: $C_5H_4N_4OS$
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: pK_{a2} 4.9; pK_{a3} 9.17 (30°, H_2O)
Other Data: Exists predominantly as 7-hydroxy tautomer in neutral soln.

>>**Variant:** *SH*-form

Molecular Formula: $C_5H_4N_4S$
Molecular Weight: 152.179
Accurate Mass: 152.015666
Percentage Composition: C 39.46%; H 2.65%; N 36.82%; S 21.07%