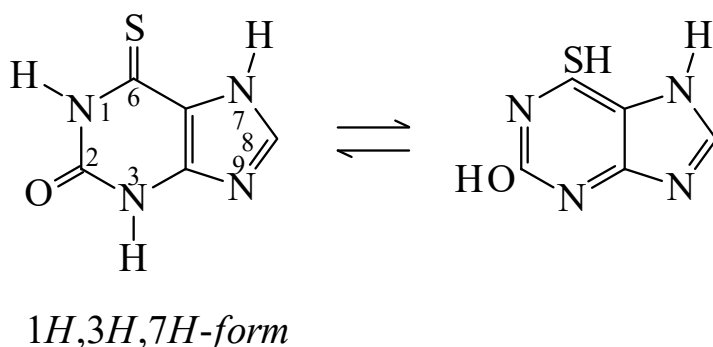




>>Entry Name: 1,3,6,7-Tetrahydro-6-thioxo-2*H*-purin-2-one

Synonym(s): 6-Thioxanthine, 8Cl. 2-Hydroxy-6-mercaptopurine



CAS Registry Number: 2002-59-7

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: Tan powder

Aldrich: 85257-0

Sigma: T8125

>>Variant: (*1H,3H,7H*)-form

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: Tan powder

>>Derivative: *N*¹-Me

Synonym(s): 1-Methyl-6-thioxanthine

Molecular Formula: C₆H₆N₄OS

Molecular Weight: 182.206

Accurate Mass: 182.026231

Percentage Composition: C 39.55%; H 3.32%; N 30.75%; O 8.78%; S 17.60%

Physical Description: Pale yellow cryst.

Melting Point: Mp 323-325 dec.°

>>Derivative: *N*³-Me

Synonym(s): 3-Methyl-6-thioxanthine

CAS Registry Number: 33285-76-6

Molecular Formula: C₆H₆N₄OS

Molecular Weight: 182.206

Accurate Mass: 182.026231

Percentage Composition: C 39.55%; H 3.32%; N 30.75%; O 8.78%; S 17.60%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 320-322 dec.°

>>Derivative: *N*⁷-Me

Synonym(s): 6-Thioheteroxanthine

CAS Registry Number: 38695-88-4

Molecular Formula: C₆H₆N₄OS

Molecular Weight: 182.206

Accurate Mass: 182.026231

Percentage Composition: C 39.55%; H 3.32%; N 30.75%; O 8.78%; S 17.60%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 343-344°