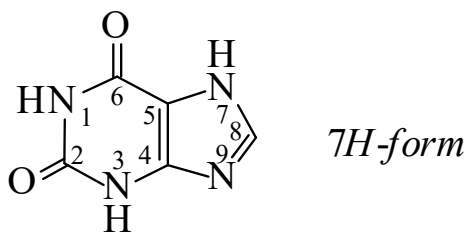




>>Entry Name: Xanthine, 8Cl

ENTRY UNDER REVIEW

Synonym(s): 3,7-Dihydro-1*H*-purine-2,6-dione, 9Cl. 2,6-Dihydroxypurine. 2,6-Purinediol



CAS Registry Number: 69-89-6

Molecular Formula: C₅H₄N₄O₂

Molecular Weight: 152.112

Accurate Mass: 152.033426

Percentage Composition: C 39.48%; H 2.65%; N 36.83%; O 21.04%

Biological Source: Found in potatoes, coffee beans, etc.

Physical Description: Cryst.

Melting Point: Mp 350°

pKa Value: p*K*_{a1} 7.7; p*K*_{a2} 11.94 (20°) p*K*_{a1} 0.8; p*K*_{a2} 7.45; p*K*_{a3} 11.13 (20°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 500 mg/kg

Aldrich: 10954-1

Fluka: 95490

>>Variant: 7*H*-form

Molecular Formula: C₅H₄N₄O₂

Molecular Weight: 152.112

Accurate Mass: 152.033426

Percentage Composition: C 39.48%; H 2.65%; N 36.83%; O 21.04%

>>Derivative: 1-Me

>>Derivative: 1-Et

CAS Registry Number: 104285-81-6

Molecular Formula: C₇H₈N₄O₂

Molecular Weight: 180.166

Accurate Mass: 180.064726

Percentage Composition: C 46.67%; H 4.48%; N 31.10%; O 17.76%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 300°

>>Derivative: 3-Me