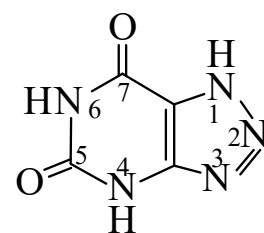




>>Entry Name: 1*H*-1,2,3-Triazolo[4,5-*d*]pyrimidine-5,7(4*H*,6*H*)-dione, 9Cl

Synonym(s): 8-Azaxanthine. Xanthazol



CAS Registry Number: 1468-26-4

Molecular Formula: C₄H₃N₅O₂

Molecular Weight: 153.1

Accurate Mass: 153.028675

Percentage Composition: C 31.38%; H 1.97%; N 45.74%; O 20.90%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 320°

Hazard & Toxicity: LD₅₀ (mus, ipr) 200 mg/kg

Fluka: 11460

Rare Chemicals Library: S42320-3

Sigma: A2132

>>Derivative: 6-Me

Molecular Formula: C₅H₅N₅O₂

Molecular Weight: 167.127

Accurate Mass: 167.044325

Percentage Composition: C 35.93%; H 3.02%; N 41.90%; O 19.15%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 262°

>>Derivative: 4,6-Di-Me

Molecular Formula: C₆H₇N₅O₂

Molecular Weight: 181.154

Accurate Mass: 181.059975

Percentage Composition: C 39.78%; H 3.89%; N 38.66%; O 17.66%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 258-260°

>>Derivative: 1,4,6-Tri-Me

Molecular Formula: C₇H₉N₅O₂

Molecular Weight: 195.18

Accurate Mass: 195.075625

Percentage Composition: C 43.08%; H 4.65%; N 35.88%; O 16.39%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 202-203°

References:

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