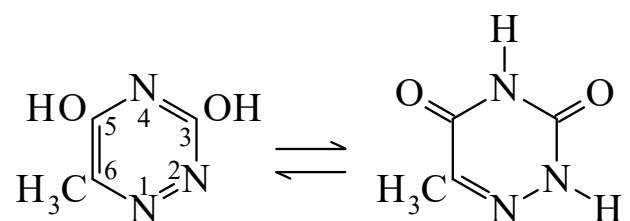




>>Entry Name: 3,5-Dihydroxy-6-methyl-1,2,4-triazine

Synonym(s): 6-Methyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione, 9Cl. 6-Azathymine



CAS Registry Number: 932-53-6

Molecular Formula: C₄H₅N₃O₂

Molecular Weight: 127.102

Accurate Mass: 127.038177

Percentage Composition: C 37.80%; H 3.96%; N 33.06%; O 25.18%

General Statement: 2*H*,4*H*-Form predominates

Use/Importance: Pyrimidine antagonist in biological systems

Physical Description: Cryst. (H₂O)

Melting Point: Mp 216° (208°)

Hazard & Toxicity: LD₅₀ (rat, ipr) 1800 mg/kg

Aldrich: 21693-3

Sigma: A1507

>>Variant: Dioxo-form

Molecular Formula: C₄H₅N₃O₂

Molecular Weight: 127.102

Accurate Mass: 127.038177

Percentage Composition: C 37.80%; H 3.96%; N 33.06%; O 25.18%

>>Derivative: 2-Me

Molecular Formula: C₅H₇N₃O₂

Molecular Weight: 141.129

Accurate Mass: 141.053827

Percentage Composition: C 42.55%; H 5.00%; N 29.77%; O 22.67%

Physical Description: Cryst.

Melting Point: Mp 200-202°

>>Derivative: 4-Me

Molecular Formula: C₅H₇N₃O₂

Molecular Weight: 141.129

Accurate Mass: 141.053827

Percentage Composition: C 42.55%; H 5.00%; N 29.77%; O 22.67%

Physical Description: Cryst.

Melting Point: Mp 155°

>>Derivative: 2,4-Di-Me

Molecular Formula: C₆H₉N₃O₂

Molecular Weight: 155.156

Accurate Mass: 155.069477

Percentage Composition: C 46.45%; H 5.85%; N 27.08%; O 20.62%

Physical Description: Cryst.

Melting Point: Mp 101-103°

>>Variant: Diol-form

Molecular Formula: C₄H₅N₃O₂

Molecular Weight: 127.102

Accurate Mass: 127.038177

Percentage Composition: C 37.80%; H 3.96%; N 33.06%; O 25.18%

Other Data: Minor tautomer