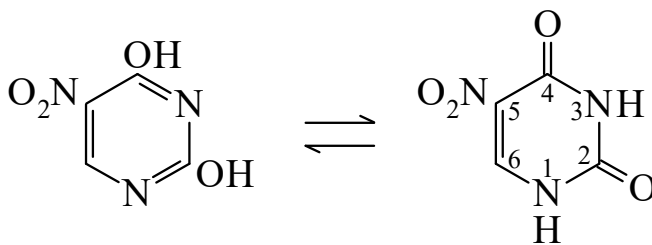




>>Entry Name: 2,4-Dihydroxy-5-nitropyrimidine

Synonym(s): 5-Nitro-2,4(1*H*,3*H*)-pyrimidinedione, 9Cl. 5-Nitrouracil. 5-Nitro-2,4-pyrimidinediol



CAS Registry Number: 611-08-5

Molecular Formula: C₄H₃N₃O₄

Molecular Weight: 157.085

Accurate Mass: 157.012357

Percentage Composition: C 30.58%; H 1.92%; N 26.75%; O 40.74%

Physical Description: Golden-yellow needles (H₂O)

Melting Point: Mp 309-311°

Aldrich: 85276-7

Fluka: 74100

Sigma: N5127

>>Variant: *NH*-form

Molecular Formula: C₄H₃N₃O₄

Molecular Weight: 157.085

Accurate Mass: 157.012357

Percentage Composition: C 30.58%; H 1.92%; N 26.75%; O 40.74%

>>Derivative: 3*N*-Me

CAS Registry Number: 25912-37-2

Molecular Formula: C₅H₅N₃O₄

Molecular Weight: 171.112

Accurate Mass: 171.028007

Percentage Composition: C 35.10%; H 2.95%; N 24.56%; O 37.40%

Physical Description: Needles (EtOH)

Melting Point: Mp 255-256°

>>Derivative: 1,3*N*-Di-Me

CAS Registry Number: 41613-26-7

Molecular Formula: C₆H₇N₃O₄

Molecular Weight: 185.139

Accurate Mass: 185.043657

Percentage Composition: C 38.93%; H 3.81%; N 22.70%; O 34.57%

Physical Description: Needles (H₂O)

Melting Point: Mp 154.5°

>>Derivative: 3*N*-Et

Molecular Formula: C₆H₇N₃O₄

Molecular Weight: 185.139

Accurate Mass: 185.043657

Percentage Composition: C 38.93%; H 3.81%; N 22.70%; O 34.57%

Physical Description: Needles (H₂O)

Melting Point: Mp 194.5°

>>Derivative: 1*N*-Me, 3*N*-Et

Molecular Formula: C₇H₉N₃O₄

Molecular Weight: 199.166

Accurate Mass: 199.059307

Percentage Composition: C 42.21%; H 4.55%; N 21.10%; O 32.13%

Physical Description: Pearly cryst. (H₂O)

Melting Point: Mp 73°