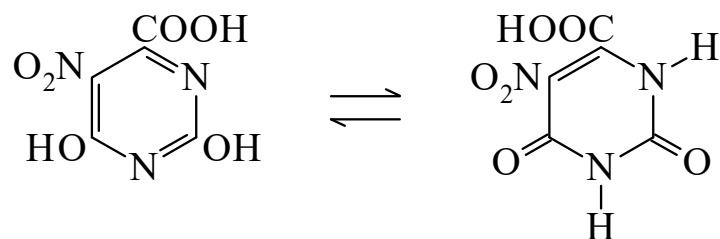




>>Entry Name: 2,6-Dihydroxy-5-nitro-4-pyrimidinecarboxylic acid

Synonym(s): 1,2,3,6-Tetrahydro-5-nitro-2,4-dioxo-6-pyrimidinecarboxylic acid, 9Cl. 5-Nitroorotic acid, 8Cl



CAS Registry Number: 17687-24-0

Related CAS Registry Numbers(s): 6311-71-3 65717-13-7 72460-04-9 83721-79-3 91838-61-8 91838-62-9 91838-63-0 91992-95-9 91992-97-1 92049-49-5

Molecular Formula: C₅H₃N₃O₆

Molecular Weight: 201.095

Accurate Mass: 201.002187

Percentage Composition: C 29.86%; H 1.50%; N 20.90%; O 47.74%

General Statement: The *NH* form is predominant

Use/Importance: Forms complexes with divalent metal-ligand species (Cu²⁺, Ni²⁺, Pd²⁺, Pt²⁺, Zn²⁺ reported)

Physical Description: Pale yellow cryst. (H₂O or EtOH)

Melting Point: Mp 230 dec.°

pKa Value: pK_{a1} 1.5 (25°) pK_{a2} 4.94 (25°)

>>Derivative: K salt

CAS Registry Number: 60779-49-9

Physical Description: Ivory-yellow cryst.

Melting Point: Mp 300°

Aldrich: 18528-0

>>Derivative: Me ester

CAS Registry Number: 6311-73-5

Molecular Formula: C₆H₅N₃O₆

Molecular Weight: 215.122

Accurate Mass: 215.017837

Percentage Composition: C 33.50%; H 2.34%; N 19.53%; O 44.62%

Physical Description: Cryst.

Melting Point: Mp 229-230°

Sigma: N8251

>>Derivative: Me ester, monohydrate

Physical Description: Cryst. (H₂O)

Melting Point: Mp 199-200 dec.°

>>Derivative: Et ester

CAS Registry Number: 52047-16-2

Molecular Formula: C₇H₇N₃O₆

Molecular Weight: 229.149

Accurate Mass: 229.033487

Percentage Composition: C 36.69%; H 3.08%; N 18.34%; O 41.89%

Melting Point: Mp 251 dec.°

Rare Chemicals Library: S78384-6

>>Variant: *OH*-form

Molecular Formula: C₅H₃N₃O₆

Molecular Weight: 201.095

Accurate Mass: 201.002187

Percentage Composition: C 29.86%; H 1.50%; N 20.90%; O 47.74%