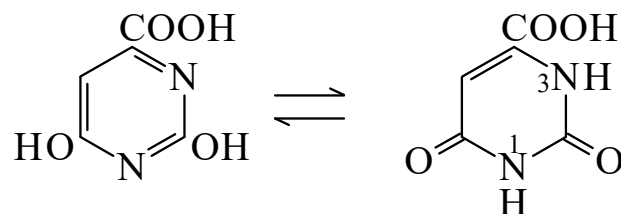




>>Entry Name: 2,6-Dihydroxy-4-pyrimidinecarboxylic acid

ENTRY UNDER REVIEW

Synonym(s): 1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid, 9CI. **Orotic acid**, BAN, INN. Uracil-6-carboxylic acid. Vitamin B₁₃. Whey factor. Many other names



CAS Registry Number: 65-86-1

Related CAS Registry Numbers(s): 154-85-8 5266-20-6 22454-86-0 24598-73-0 50887-69-9

Type of Compound Code(s): WK4000 WI6000 PA4950 PS8300 VX6960 XA6850 WK6000

Molecular Formula: C₅H₄N₂O₄

Molecular Weight: 156.098

Accurate Mass: 156.017108

Percentage Composition: C 38.47%; H 2.58%; N 17.95%; O 41.00%

General Statement: Intermediate tautomers also possible. Exists as the dioxo tautomer in the cryst. state

Biological Source: Occurs in milk and other biol. systems

Use/Importance: Key compd. involved in biosynth. of nucleic acid pyrimidine bases. Shows bacteriostatic and cytostatic props. Forms metal complexes. Uricosuric agent.

Used in photometric detn. of Zn

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 322-325°. Mp 345-346°

pKa Value: pK_{a1} 1.8; pK_{a2} 9.55 (25°)

Calculated Log P Data: Log P -0.75 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 2000 mg/kg

Fluka: 75500

Sigma: O1756

>>Derivative: Me ester

CAS Registry Number: 6153-44-2

Molecular Formula: C₆H₆N₂O₄

Molecular Weight: 170.124

Accurate Mass: 170.032758

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Physical Description: Cryst.

Melting Point: Mp 240-242°. Mp 249°

pKa Value: pK_{a1} 7.93 (25°)

Sigma: O3627

>>Derivative: Et ester

CAS Registry Number: 1747-53-1

Molecular Formula: C₇H₈N₂O₄

Molecular Weight: 184.151

Accurate Mass: 184.048408

Percentage Composition: C 45.66%; H 4.38%; N 15.21%; O 34.75%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 207-208°

>>Derivative: Propyl ester

CAS Registry Number: 4450-26-4

Molecular Formula: C₈H₁₀N₂O₄

Molecular Weight: 198.178

Accurate Mass: 198.064058

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

Physical Description: Cryst.

Melting Point: Mp 234-236°