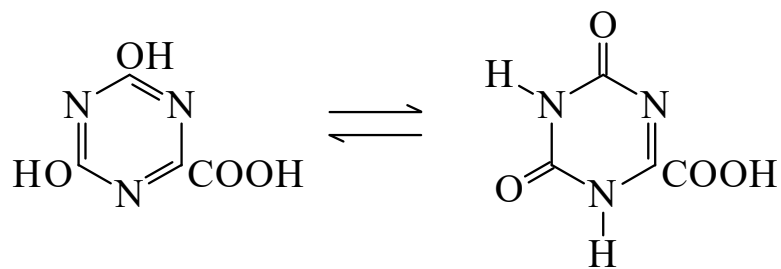




>>Entry Name: Oteracil, INN

Synonym(s): 1,4,5,6-Tetrahydro-4,6-dioxo-1,3,5-triazine-2-carboxylic acid, 9Cl. 4,6-Dihydroxy-1,3,5-triazine-2-carboxylic acid. Allantoxanic acid, 8Cl. 5-Azaorotic acid. Oxonic acid



CAS Registry Number: 937-13-3

Related CAS Registry Numbers(s): 2207-75-2

Molecular Formula: $C_4H_3N_3O_4$

Molecular Weight: 157.085

Accurate Mass: 157.012357

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

Other Data: Free acid v. unstable. Component (as K salt) of S1, a new oral formulation of Tegafor [BNH54-X](#)

>>Derivative: Amide

CAS Registry Number: 69391-08-8

Molecular Formula: $C_4H_4N_4O_3$

Molecular Weight: 156.101

Accurate Mass: 156.028341

Percentage Composition: C 30.78%; H 2.58%; N 35.89%; O 30.75%

Melting Point: Mp 350°

Other Data: Darkens >300°

Sigma: A0778

References:

- Brandenburger, H. *et al.*, *Helv. Chim. Acta*, 1954, **37**, 641; 2207, (*synth*)
Piskala, A. *et al.*, *Coll. Czech. Chem. Comm.*, 1962, **27**, 1562; 1572, (*synth*)
Pike, R.K., *Org. Magn. Reson.*, 1976, **8**, 224, (*struct*)
Piskala, A. *et al.*, *Nucleic Acid Chem.*, 1978, **1**, 93, (*synth*)
Shirasaka, T. *et al.*, *Cancer Res.*, 1993, **53**, 4004-4009, (*pharmacol*)
Takechi, T. *et al.*, *Cancer Chemother. Pharmacol.*, 1997, **39**, 205-211, (*pharmacol*)