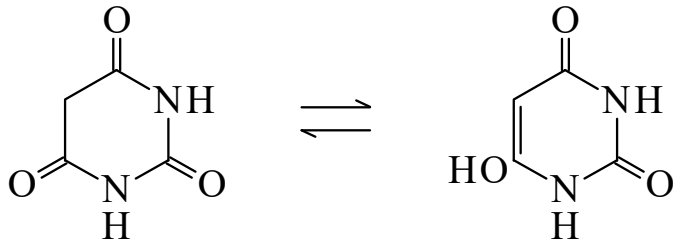
>>**Entry Name: 2,4,6(1*H*,3*H*,5*H*)-Pyrimidinetrione,** 9CI
Synonym(s): Barbituric acid, 8CI. Malonylurea



CAS Registry Number: 67-52-7

Molecular Formula: $C_4H_4N_2O_3$
Molecular Weight: 128.087
Accurate Mass: 128.022193
Percentage Composition: C 37.51%; H 3.15%; N 21.87%; O 37.47%

Use/Importance: Used in plastic manuf. and in photometric detn. of $CN^{(-)}$ and $Cl^{(-)}$. Parent compd. of the barbiturate sedatives but is said to have no sedative props.
Physical Description: Dihydrate, prisms (H_2O)
Melting Point: Mp 248 dec.°
Hazard & Toxicity: LD_{50} (rat, orl) >5000 mg/kg

Aldrich: B20-8
Fluka: 11710
Sigma: B0625

>>**Derivative:** *N*-Me
Synonym(s): 1-Methyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9CI. 1-Methylbarbituric acid

CAS Registry Number: 2565-47-1
Molecular Formula: $C_5H_6N_2O_3$
Molecular Weight: 142.114
Accurate Mass: 142.037843
Percentage Composition: C 42.26%; H 4.26%; N 19.71%; O 33.77%
Physical Description: Plates (EtOH)
Melting Point: Mp 132°
pKa Value: pK_a 4.35 (25°)

>>**Derivative:** 1,3-Di-Me
Synonym(s): 1,3-Dimethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9CI. 1,3-Dimethylbarbituric acid. Malonyldimethylurea

CAS Registry Number: 769-42-6

Molecular Formula: $C_6H_8N_2O_3$
Molecular Weight: 156.141
Accurate Mass: 156.053493
Percentage Composition: C 46.15%; H 5.16%; N 17.94%; O 30.74%
Use/Importance: Used for photometric detn. of $CN^{(-)}$ (λ_{max} 588 nm)
Physical Description: Needles
Melting Point: Mp 123°
Solubility: Sol. H_2O
pKa Value: pK_{a1} 4.68 (25°)
Other Data: Sublimes
Aldrich: 31800-0
Fluka: 39565

>>**Derivative:** *N*-Et

CAS Registry Number: 50721-57-8
Molecular Formula: $C_6H_8N_2O_3$
Molecular Weight: 156.141
Accurate Mass: 156.053493
Percentage Composition: C 46.15%; H 5.16%; N 17.94%; O 30.74%
Physical Description: Rectangular leaflets (EtOH)
Melting Point: Mp 119-120°