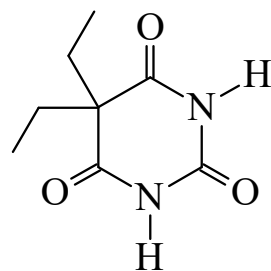




>>Entry Name: **Barbital**, INN

Synonym(s): 5,5-Diethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9CI. 5,5-Diethylbarbituric acid. Diethylmalonylurea. Barbitone, BAN. Veronal. Many other names



CAS Registry Number: 57-44-3

Molecular Formula: C₈H₁₂N₂O₃

Molecular Weight: 184.194

Accurate Mass: 184.084793

Percentage Composition: C 52.17%; H 6.57%; N 15.21%; O 26.06%

General Statement: Exists in several tautomeric forms

Biological Source: Isol. from tissues of the Indian puffer fish *Sphaeroides oblongus*

Use/Importance: Powerful hypnotic and sedative of long duration

Physical Description: Faintly bitter cryst. (H₂O); polymorphic forms; trigonal cryst., monoclinic prisms, monoclinic needles, triclinic cryst.

Melting Point: Mp 190°. Mp 183° (181°, 176°)

pKa Value: p*K*_{a1} 8.02 (25°) p*K*_a 7.43

Calculated Log P Data: Log P 0.66 (calc)

UV: [neutral] λ_{max} 224 () (EtOH) (Berdy) [base] λ_{max} 224 (); 240 () (EtOH-NaOH) (Berdy) [base] λ_{max} 243 () (NaOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 600 mg/kg

Fluka: 32000

Sigma: B8632

>>Derivative: Na salt

Synonym(s): **Barbital sodium**, INN

CAS Registry Number: 144-02-5

Hazard & Toxicity: Fatal in large doses. LD₅₀ (rat, orl) 600 mg/kg. Exp. reprod. and teratogenic effects

Fluka: 32002

Sigma: B0500

>>Derivative: *N*-Me

see Metharbital, [DKP96-A](#)

>>Derivative: *N*-Isopropyl

CAS Registry Number: 85432-35-5

Molecular Formula: C₁₁H₁₈N₂O₃

Molecular Weight: 226.275

Accurate Mass: 226.131743

Percentage Composition: C 58.39%; H 8.02%; N 12.38%; O 21.21%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 116°

>>Derivative: *N*¹,*N*³-Di-Me

CAS Registry Number: 714-59-0

Molecular Formula: C₁₀H₁₆N₂O₃

Molecular Weight: 212.248

Accurate Mass: 212.116093

Percentage Composition: C 56.59%; H 7.60%; N 13.20%; O 22.61%

Physical Description: Cryst.

Melting Point: Mp 37°