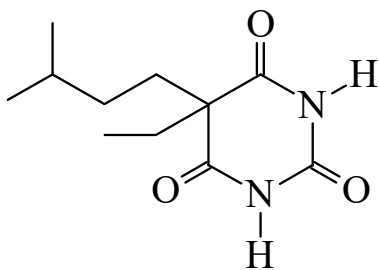




>>Entry Name: Amobarbital, INN, USAN

Synonym(s): 5-Ethyl-5-(3-methylbutyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9Cl. 5-Ethyl-5-isopentylbarbituric acid. Amylobarbitone, BAN. Amital. Pentymal



CAS Registry Number: 57-43-2

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%

Use/Importance: Sedative, narcotic

Physical Description: Leaflets (H₂O or EtOH aq.)

Melting Point: Mp 156-158°

pKa Value: p*K*_{a1} 7.96 (25°)

Calculated Log P Data: Log P 2.11 (calc)

Hazard & Toxicity: CNS depressant. LD₅₀ (rat, orl) 250 mg/kg

Sigma: A5255

>>Derivative: Na salt

Synonym(s): Amobarbital sodium, USAN. Talamo. Amytal sodium. Barbamyl

CAS Registry Number: 64-43-7

Other Data: Component of Tuinal

Hazard & Toxicity: LD₅₀ (rat, orl) 275 mg/kg

Sigma: A4430

References:

Shonle, H.A. *et al.*, *J.A.C.S.*, 1923, **45**, 246, (*synth*)

Maynert, E.W. *et al.*, *J.O.C.*, 1950, **15**, 259, (*synth*)

Tsuruta, M. *et al.*, *Nippon Kagaku Kaishi*, 1951, **54**, 722, (*synth*)

Grützmacher, H.F. *et al.*, *Tet. Lett.*, 1966, 1365, (*ms*)

Craven, B.M. *et al.*, *J. Mol. Struct.*, 1973, **16**, 331, (*cryst struct*)

Okada, J. *et al.*, *Chem. Pharm. Bull.*, 1974, **22**, 1580, (*cmr*)

Mian, N.A.A. *et al.*, *Anal. Profiles Drug Subst.*, 1990, **19**, 27, (*rev*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 565

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AMX750; AON750