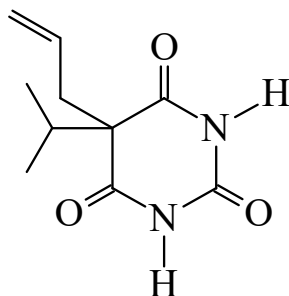




>>Entry Name: Aprobarbital, INN

Synonym(s): 5-(1-Methylethyl)-5-(2-propenyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9Cl. 5-Allyl-5-isopropylbarbituric acid. Alurate. Numal. Isonal. Aprozal. Allonal. Somnipron. Many other names



CAS Registry Number: 77-02-1

Molecular Formula: C₁₀H₁₄N₂O₃

Molecular Weight: 210.232

Accurate Mass: 210.100443

Percentage Composition: C 57.13%; H 6.71%; N 13.32%; O 22.83%

Biological Use/Importance: Sedative, hypnotic

Physical Description: Cryst.

Melting Point: Mp 140-141.5°

Calculated Log P Data: Log P 1.1 (calc)

Other Data: Polymorphic forms known

Hazard & Toxicity: LD₅₀ (mus, ipr) 200 mg/kg

Sigma: A7023

>>Derivative: Na salt

CAS Registry Number: 125-88-2

Physical Description: Hygroscopic powder

Hazard & Toxicity: LD₅₀ (rat, ipr) 85 mg/kg

>>Derivative: N¹-Me

Synonym(s): 1-Methyl-5-(1-methylethyl)-5-(2-propenyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9Cl. 5-Allyl-5-isopropyl-1-methylbarbituric acid. Enallylpropymal. Narconumal

CAS Registry Number: 1861-21-8

Molecular Formula: C₁₁H₁₆N₂O₃

Molecular Weight: 224.259

Accurate Mass: 224.116093

Percentage Composition: C 58.91%; H 7.19%; N 12.49%; O 21.40%

Melting Point: Mp 56-57°

Boiling Point: Bp₁₂ 176-178°

Calculated Log P Data: Log P 1.59 (calc)

References:

U.S. Pat., 1923, 1 444 802

U.K. Pat., 1937, *Hoffmann-La Roche*, 454 779; *CA*, **31**, 1555⁷, (*synth*, *N-Me*)

Sandberg, F., *Acta Physiol. Scand.*, 1949, **18**, 204, (*pharmacol*)

Gräfe, H.J. *et al.*, *Arzneim.-Forsch.*, 1958, **8**, 293, (*activity*)

Hansch, C. *et al.*, *J. Med. Chem.*, 1967, **10**, 745, (*biol activity*)

Fales, H.M. *et al.*, *Arch. Mass Spectral Data*, 1971, **2**, 580, (*ms*)

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

Rae, A.D., *Cryst. Struct. Commun.*, 1975, **4**, 457, (*cryst struct*)

Harvey, D.J. *et al.*, *Drug Metab. Dispos.*, 1977, **5**, 527, (*metab*)

Yih, T.D. *et al.*, *J. Pharmacol. Exp. Ther.*, 1977, **203**, 184, (*pharmacol*)

Martindale, The Extra Pharmacopoeia, 30th edn., *Pharmaceutical Press*, 1993, 566

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 7th edn., *Akademie-Verlag*, 1994, 1998, (*synonyms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, AFT000; BOQ750