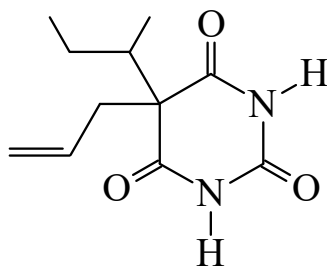




>>Entry Name: Talbutal, INN, USAN

Synonym(s): 5-(1-Methylpropyl)-5-(2-propenyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9Cl. 5-Allyl-5-*sec*-butylbarbituric acid, 8Cl. Lutawin. Lotusate. Profundol



CAS Registry Number: 115-44-6

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%

Use/Importance: Sedative, hypnotic

Calculated Log P Data: Log P 1.63 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 57.5 mg/kg

>>Variant: (±)-form

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 108-110°

pKa Value: pK_a 7.9 (20°)

References:

Volwiler, E.H., *J.A.C.S.*, 1925, **47**, 2236, (*synth*)

Parker, K.D. *et al.*, *Anal. Chem.*, 1961, **33**, 1378, (*glc*)

Goenechea, S., *Z. Anorg. Allg. Chem.*, 1966, **218**, 416, (*ir*)

Avdovich, H.W. *et al.*, *Can. J. Pharm. Sci.*, 1969, **4**, 51, (*pmr*)

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

Schentz, C. *et al.*, *Dtsch. Apoth. -Ztg.*, 1973, **113**, 1553, (*tlc*)

Siek, T.J. *et al.*, *J. Forensic Sci.*, 1975, **20**, 18, (*uv*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 616

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AFY500