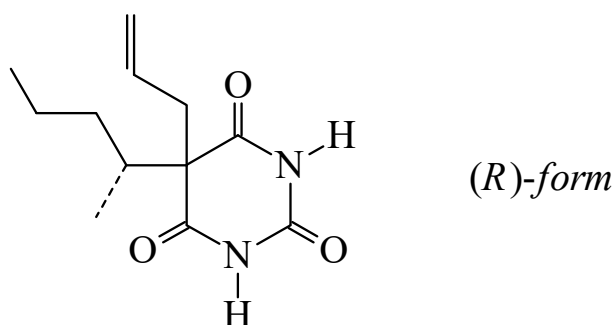




>>Entry Name: Quinalbarbitone

Synonym(s): 5-(1-Methylbutyl)-5-(2-propenyl)-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9Cl. 5-Allyl-5-(1-methylbutyl)barbituric acid, 8Cl. Secobarbitone. **Secobarbital**, INN, USAN. Ional. Quinalbarbital



CAS Registry Number: 76-73-3

Molecular Formula: C₁₂H₁₈N₂O₃

Molecular Weight: 238.286

Accurate Mass: 238.131743

Percentage Composition: C 60.49%; H 7.61%; N 11.76%; O 20.14%

Use/Importance: Sedative

Calculated Log P Data: Log P 2.16 (calc)

Hazard & Toxicity: Adverse, dose-related, CNS effects reported when used therapeutically. LD₅₀ (mus, orl) 145 mg/kg

Sigma: S4006

>>Variant: (*R*)-form

CAS Registry Number: 22328-94-5

Molecular Formula: C₁₂H₁₈N₂O₃

Molecular Weight: 238.286

Accurate Mass: 238.131743

Percentage Composition: C 60.49%; H 7.61%; N 11.76%; O 20.14%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 103-106°

Optical Rotation: $[\alpha]_D^{22} +9.23$ (c, 2 in EtOH)

>>Variant: (*S*)-form

Molecular Formula: C₁₂H₁₈N₂O₃

Molecular Weight: 238.286

Accurate Mass: 238.131743

Percentage Composition: C 60.49%; H 7.61%; N 11.76%; O 20.14%

Physical Description: Cryst. by subl.

Melting Point: Mp 102.5-103.5°

Optical Rotation: $[\alpha]_D^{24} -8.55$ (c, 2.3 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 29071-21-4

Molecular Formula: C₁₂H₁₈N₂O₃

Molecular Weight: 238.286

Accurate Mass: 238.131743

Percentage Composition: C 60.49%; H 7.61%; N 11.76%; O 20.14%

Physical Description: Cryst.

Melting Point: Mp 98-100°

pKa Value: pK_a 12.6

>>Derivative: Na salt

Synonym(s): Quinalbarbitone sodium, BAN. Secobarbital sodium, INN. Seconal sodium. Tuinal

CAS Registry Number: 309-43-3

Physical Description: Hygroscopic powder

Hazard & Toxicity: Absorbed through skin. LD₅₀ (rat, orl) 125 mg/kg

Sigma: S1378