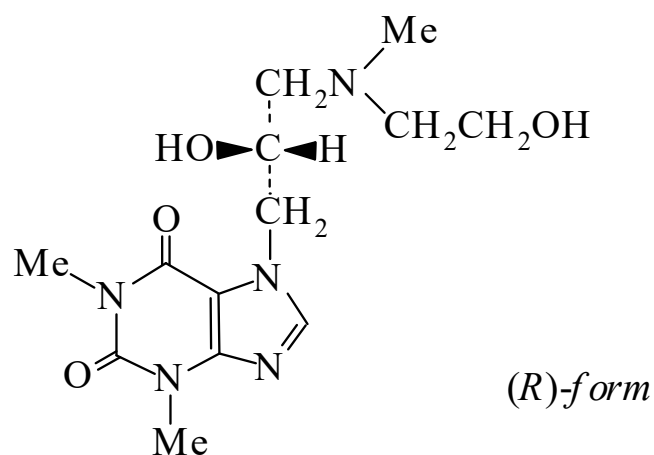




>>Entry Name: Xanthinol

Synonym(s): 3,7-Dihydro-7-[2-hydroxy-3-[(2-hydroxyethyl)methylamino]propyl]-1,3-dimethyl-1*H*-purine-2,6-dione, 9Cl. 7-[2-Hydroxy-3-[(2-hydroxyethyl)methylamino]propyl]theophylline, 8Cl. Xanthinol. Metoxiprofilin. Many other names



CAS Registry Number: 2530-97-4

Molecular Formula: C₁₃H₂₁N₅O₄

Molecular Weight: 311.34

Accurate Mass: 311.159355

Percentage Composition: C 50.15%; H 6.80%; N 22.49%; O 20.56%

Use/Importance: Peripheral vasodilator, low acute toxicity

Calculated Log P Data: Log P -1.39 (uncertain value) (calc)

>>Variant: (R)-form

Molecular Formula: C₁₃H₂₁N₅O₄

Molecular Weight: 311.34

Accurate Mass: 311.159355

Percentage Composition: C 50.15%; H 6.80%; N 22.49%; O 20.56%

Physical Description: Cryst. (Me₂CO/pentane)

Melting Point: Mp 87-88°

Optical Rotation: [α]_D²⁰ -76.54 (c, 8.1 in EtOH)

>>Variant: (±)-form

Molecular Formula: C₁₃H₂₁N₅O₄

Molecular Weight: 311.34

Accurate Mass: 311.159355

Percentage Composition: C 50.15%; H 6.80%; N 22.49%; O 20.56%

>>Derivative: Nicotinate salt

Synonym(s): Xanthinol nicotinate, BAN. Xanthinol niacinate, USAN. Xanthinol nicotinate, INN. Complamin. Xavin

CAS Registry Number: 437-74-1

Melting Point: Mp 180°

Solubility: Sol. H₂O

Hazard & Toxicity: Exp. reprod. and teratogenic effects

>>Derivative: Compd. with clofibric acid

Synonym(s): Xantifibrate, INN

CAS Registry Number: 36921-54-7

References: