



>>Derivative: 1,3-Di-Me

>>Derivative: 1,7-Di-Me

Synonym(s): 3,7-Dihydro-1,7-dimethyl-1*H*-purine-2,6-dione, 9Cl. Paraxanthine. 1,7-Dimethylxanthine

CAS Registry Number: 611-59-6

Molecular Formula: C₇H₈N₄O₂

Molecular Weight: 180.166

Accurate Mass: 180.064726

Percentage Composition: C 46.67%; H 4.48%; N 31.10%; O 17.76%

Biological Source: Present in human urine

Physical Description: Plates (H₂O)

Melting Point: Mp 298-299°

pKa Value: p*K*_{a1} 8.6

Aldrich: 27151-9

Fluka: 41761

Sigma: D5385

>>Derivative: 3,7-Di-Me

>>Derivative: 1,3,7-Tri-Me

>>Derivative: 3-Propyl

Synonym(s): 3,7-Dihydro-3-propyl-1*H*-purine-2,6-dione, 9Cl. 3-Propylxanthine. **Enprofylline**, INN, USAN. Nilyph. Oxeze. D 4028

CAS Registry Number: 41078-02-8

Molecular Formula: C₈H₁₀N₄O₂

Molecular Weight: 194.193

Accurate Mass: 194.080376

Percentage Composition: C 49.48%; H 5.19%; N 28.85%; O 16.48%

Use/Importance: Diuretic, antiasthmatic agent, bronchodilator. Lacks adenosine receptor antagonism of Xanthine

Melting Point: Mp 287-289°

Calculated Log P Data: Log P 0.36 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 481 mg/kg

Fluka: 82480

Sigma: P5679

>>Derivative: 1,3-Dipropyl, 7-Me

Synonym(s): 3,7-Dihydro-7-methyl-1,3-dipropyl-1*H*-purine-2,6-dione, 9Cl

CAS Registry Number: 31542-63-9

Molecular Formula: C₁₂H₁₈N₄O₂

Molecular Weight: 250.3

Accurate Mass: 250.142976

Percentage Composition: C 57.58%; H 7.25%; N 22.38%; O 12.78%

Use/Importance: Adenoside A₂-antagonist. Depressant

Physical Description: Cryst. (Me₂CO/DMF)

Melting Point: Mp 116°