>>**Derivative:** 1,3-Di-Me

>>**Derivative:** 1,7-Di-Me
Synonym(s): 3,7-Dihydro-1,7-dimethyl-1*H*-purine-2,6-dione, 9CI. Paraxanthine. 1,7-Dimethylxanthine

CAS Registry Number: 611-59-6

Molecular Formula: $C_7H_8N_4O_2$
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 (H_2O)
Melting Point: Mp 298-299°
pKa Value: pK_{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, 9CI. 3-Propylxanthine. **Enprofylline,** INN, USAN**.** Nilyph. Oxeze. D 4028

CAS Registry Number: 41078-02-8

Molecular Formula: $C_8H_{10}N_4O_2$
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: LD_{50} (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, 9CI

CAS Registry Number: 31542-63-9

Molecular Formula: $C_{12}H_{18}N_4O_2$
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 A_2-antagonist. Depressant
Physical Description: Cryst. (Me_2CO/DMF)
Melting Point: Mp 116°