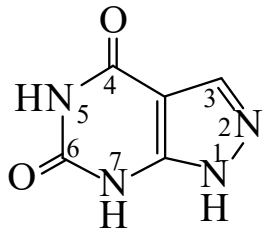
>>**Entry Name: 1*H*-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione,** 9CI
Synonym(s): Oxypurinol, BAN, USAN**.** Oxipurinol, INN. **Alloxanthine‡.** Oxoallopurinol. BW 55-5. NSC 76239



1*H-form*

CAS Registry Number: 2465-59-0

Molecular Formula: $C_5H_4N_4O_2$
Molecular Weight: 152.112
Accurate Mass: 152.033426
Percentage Composition: C 39.48%; H 2.65%; N 36.83%; O 21.04%

Source/Synthesis: Metab. of 1*H*-Pyrazolo[3,4-*d*]pyrimidin-4-ol CBX00-L
Use/Importance: Specific inhibitor of the reduced form of xanthine oxidase. Reagent for the spectrophotometric anal. of 1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane BGW21-L in pharmaceuticals
Physical Description: Cryst. (H_2O)
Melting Point: Mp 300°

Sigma: C6881

>>**Variant:** 1*H*-form

Molecular Formula: $C_5H_4N_4O_2$
Molecular Weight: 152.112
Accurate Mass: 152.033426
Percentage Composition: C 39.48%; H 2.65%; N 36.83%; O 21.04%

>>**Derivative:** 1,5-Di-Me

CAS Registry Number: 7254-33-3
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%
Physical Description: Granules
Melting Point: Mp 297-298°

>>**Derivative:** 5,7-Di-Me

CAS Registry Number: 4680-51-7
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%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 280-281°
pKa Value: pK_{a1} 9.26 (20°)

>>**Derivative:** 1,5,7-Tri-Me

CAS Registry Number: 4318-52-9
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%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 202-204°