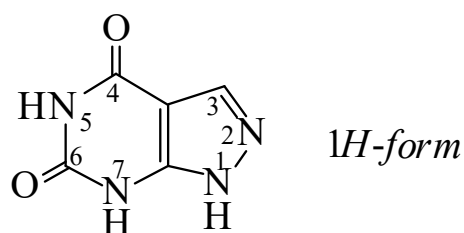




>>Entry Name: **1H-Pyrazolo[3,4-*d*]pyrimidine-4,6(5*H*,7*H*)-dione**, 9CI

Synonym(s): **Oxypurinol**, BAN, USAN. Oxipurinol, INN. **Alloxanthine**†. Oxoallopurinol. BW 55-5. NSC 76239



CAS Registry Number: 2465-59-0

Molecular Formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>

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<sup>3,7</sup>]decane [BGW21-L](#) in pharmaceuticals

Physical Description: Cryst. (H<sub>2</sub>O)

Melting Point: Mp 300°

Sigma: C6881

>>Variant: 1*H*-form

Molecular Formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>

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<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>

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<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>

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: p*K*<sub>a1</sub> 9.26 (20°)

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

CAS Registry Number: 4318-52-9

Molecular Formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>

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°