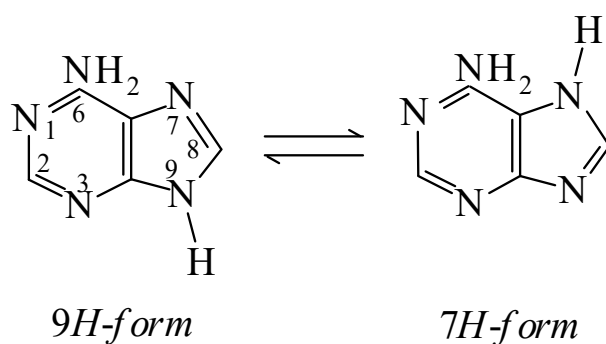




>>Entry Name: Adenine, JAN, USAN

Synonym(s): 1*H*-Purin-6-amine, 9Cl. 6-Aminopurine. Vitamin B<sub>4</sub>



CAS Registry Number: 73-24-5

Related CAS Registry Numbers(s): 2312-73-4 6055-72-7

Molecular Formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>

Molecular Weight: 135.128

Accurate Mass: 135.054495

Percentage Composition: C 44.44%; H 3.73%; N 51.83%

General Statement: 9*H*-form is favoured in free base. CAS refers mainly to 1*H* struct. which is not in reality a favoured tautomer

Biological Source: Widespread throughout animal and plant tissue, purine components, of DNA, RNA, and coenzymes and biosynthetic intermed.

Biological Use/Importance: Antiviral agent, granulocyte antagonist. Vitamin. Pharmaceutical aid used to extend storage life of whole blood

Physical Description: Needles + 3H<sub>2</sub>O (H<sub>2</sub>O)

Melting Point: Mp 360-365 (anhyd.) dec.°

pKa Value: pK<sub>a1</sub> 4.12; pK<sub>a2</sub> 9.83 (25°)

Hazard & Toxicity: Exp. reprod. and teratogenic effects. LD<sub>50</sub> (rat, orl) 745 mg/kg

Aldrich: 10496-5

Fluka: 1830

Sigma: A8626

>>Derivative: Hydrochloride

CAS Registry Number: 2922-28-3

Physical Description: Cryst. + 0.5H<sub>2</sub>O

Melting Point: Mp 285°

Fluka: 1840

Other: PB A11396

>>Derivative: Sulfate

CAS Registry Number: 321-30-2

Extra CAS Registry Numbers(s): 6509-19-9

Melting Point: Mp 285 dec.°

Aldrich: 14581-5

Fluka: 1880

Sigma: A2545

>>Derivative: *N*<sup>1</sup>-Oxide

CAS Registry Number: 700-02-7

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

Molecular Weight: 151.127

Accurate Mass: 151.04941

Percentage Composition: C 39.74%; H 3.33%; N 46.34%; O 10.59%

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

Melting Point: Mp 297-307 dec.°

Hazard & Toxicity: Exp. neoplastic agent

Rare Chemicals Library: S54066-8

Sigma: A8876