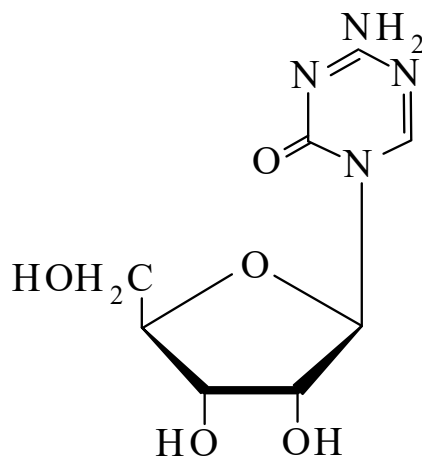




>>Entry Name: 5-Azacytidine

Synonym(s): 4-Amino-1-β-D-ribofuranosyl-1,3,5-triazin-2(1*H*)-one, 9Cl. 1-β-D-Ribofuranosyl-5-azacytosine. Ladakamycin. **Azacitidine**, INN, USAN. NSC 102816. U 18496. Antibiotic U 18496. Mylosar



CAS Registry Number: 320-67-2

Related CAS Registry Numbers(s): 52934-49-3

Molecular Formula: C₈H₁₂N₄O₅

Molecular Weight: 244.207

Accurate Mass: 244.080771

Percentage Composition: C 39.35%; H 4.95%; N 22.94%; O 32.76%

General Statement: Nucleoside antibiotic

Biological Source: Isol. from *Streptovorticillium ladakanus*, *Actinoplanes awajinensis* and *Actinoplanes missouriensis*

Use/Importance: Inhibits pyrimidine biosynthesis; antineoplastic agent. Used to treat acute non-lymphoblastic leukaemia

Development Status: No longer marketed

Melting Point: Mp 232-234 dec.°

Optical Rotation: [α]_D²⁵+39 (c, 1 in H₂O)

Solubility: BERDY SOL: Sol. H₂O; poorly sol. MeOH, hexane, DMSO

Calculated Log P Data: Log P -4 (calc)

UV: [neutral] λ_{max} (H₂O) (Berdy) [acid] λ_{max} (HCl) (Berdy) [base] λ_{max} (NaOH) (Berdy)

Hazard & Toxicity: Human systemic effects when used therapeutically. Exp. neoplastic agent. Exp. reprod. and teratogenic effects. LD₅₀ (mus, orl) 572 mg/kg ; BERDY HAZD : LD₅₀ (mus, ipr) 115 mg/kg

Aldrich: 85288-0

Fluka: 11385

Sigma: A2385

>>Derivative: 4-*N*-Me

Molecular Formula: C₉H₁₄N₄O₅

Molecular Weight: 258.233

Accurate Mass: 258.096421

Percentage Composition: C 41.86%; H 5.46%; N 21.70%; O 30.98%

Melting Point: Mp 148-150°

>>Derivative: 4-*N*-Di-Me

Molecular Formula: C₁₀H₁₆N₄O₅

Molecular Weight: 272.26

Accurate Mass: 272.112071

Percentage Composition: C 44.12%; H 5.92%; N 20.58%; O 29.38%

Melting Point: Mp 128-130°

>>Derivative: 2',3',5'-Tribenzoyl

CAS Registry Number: 28998-36-9

Molecular Formula: C₂₉H₂₄N₄O₈

Molecular Weight: 556.531

Accurate Mass: 556.159416

Percentage Composition: C 62.59%; H 4.35%; N 10.07%; O 23.00%

Melting Point: Mp 186-187°

Optical Rotation: [α]_D²⁰-33.1 (c, 1 in CHCl₃)