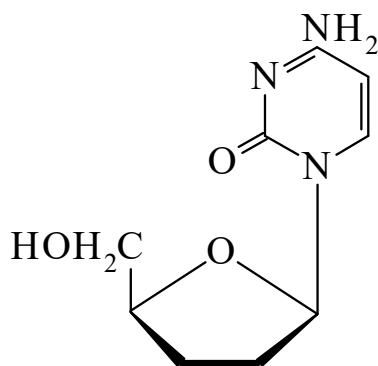




>>Entry Name: Zalcitabine, BAN, INN, USAN

Synonym(s): 2',3'-Dideoxycytidine, 9Cl. DDC. Hivid. Ro 24-2027. NSC 606170



CAS Registry Number: 7481-89-2

Molecular Formula: $C_9H_{13}N_3O_3$

Molecular Weight: 211.22

Accurate Mass: 211.095692

Percentage Composition: C 51.18%; H 6.20%; N 19.89%; O 22.72%

Use/Importance: Antiviral agent. Reverse transcriptase inhibitor. Orally active dideoxynucleoside used in combination with Zidovudine [HHQ23-E](#) for treatment of HIV infection. Nucleoside transporter substrate

Development Status: Launched 1992 (Austria)

Melting Point: Mp 231-232° (214-217°)

Optical Rotation: $[\alpha]_D^{20} +90$ (c, 0.5 in H_2O). $[\alpha]_D +105.9$ (c, 0.53 in MeOH)

Calculated Log P Data: Log P -1.32 (calc)

Aldrich: 30835-8

Sigma: D5782

>>Derivative: N-Benzoyl

Synonym(s): N^4 -Benzoyl-2',3'-dideoxycytidine

Molecular Formula: $C_{16}H_{17}N_3O_4$

Molecular Weight: 315.328

Accurate Mass: 315.121907

Percentage Composition: C 60.94%; H 5.43%; N 13.33%; O 20.30%

Use/Importance: Anti-HIV agent

Physical Description: Cryst. (EtOAc/MeOH)

>>Derivative: 5'-Triphosphate

CAS Registry Number: 66004-77-1

Molecular Formula: $C_9H_{16}N_3O_{12}P_3$

Molecular Weight: 451.16

Accurate Mass: 450.994688

Percentage Composition: C 23.96%; H 3.57%; N 9.31%; O 42.56%; P 20.60%

Use/Importance: Metab. of parent compd.

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