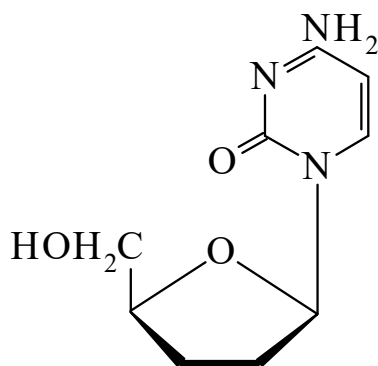




>>Entry Name: Zalcitabine, BAN, INN, USAN

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



CAS Registry Number: 7481-89-2

Molecular Formula: C₉H₁₃N₃O₃

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: [α]_D²⁰ +90 (c, 0.5 in H₂O). [α]_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): N⁴-Benzoyl-2',3'-dideoxycytidine

Molecular Formula: C₁₆H₁₇N₃O₄

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: C₉H₁₆N₃O₁₂P₃

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.

References:

- Horwitz, J.P. *et al.*, *J.O.C.*, 1967, **32**, 817, (*synth*)
Sanger, F. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 5463-5467, (*5'-triphosphate*)
Mitsuya, H. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, (London), 1986, **83**, 1911, (*pharmacol*)
Starnes, M.C. *et al.*, *J. Biol. Chem.*, 1987, **262**, 988-991, (*5'-triphosphate*)
Mitsuya, H. *et al.*, *Nature (London)*, 1987, **325**, 773
Okabe, M. *et al.*, *J.O.C.*, 1988, **53**, 4780, (*synth, ir, pmr, ms*)
Japan. Pat., 1988, 63 130 599; *CA*, **109**, 231472r, (*5'-triphosphate, synth*)
Plagemann, P.G. *et al.*, *Biochem. Pharmacol.*, 1989, **38**, 3469-3475, (*pharmacol*)
Kaskar, B. *et al.*, *J. Het. Chem.*, 1989, **26**, 1531, (*synth*)
Chu, C.K. *et al.*, *J.O.C.*, 1989, **54**, 2217, (*synth*)
Montauria, M.S. *et al.*, *Annalen*, 1990, 599, (*synth*)
Johansen, O. *et al.*, *Aust. J. Chem.*, 1991, **44**, 37, (*synth*)
Whittington, R. *et al.*, *Drugs*, 1992, **44**, 656, (*rev*)
Manchand, P.S. *et al.*, *J.O.C.*, 1992, **57**, 3473, (*synth, uv, ir, pmr, cmr*)
Gulbis, J.M. *et al.*, *Acta Cryst. C*, 1993, **49**, 1095, (*cryst struct, deriv*)
Drugs of Today (Barcelona), 1993, **29**, 19, (*rev*)
Lipsky, J.J., *Lancet*, 1993, **341**, 30
Adkins, J.C. *et al.*, *Drugs*, 1997, **53**, 1054-1080, (*rev*)