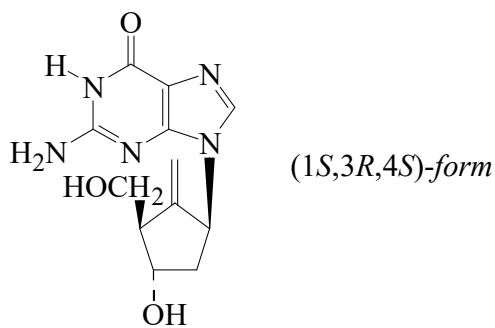




>>Entry Name: Entecavir, INN, USAN

Synonym(s): 2-Amino-1,9-dihydro-9-[4-hydroxy-3-(hydroxymethyl)-2-methylenecyclopentyl]-6*H*-purin-6-one, 9Cl. BMS 200475. SQ 34676



Related CAS Registry Numbers(s): 188399-46-4

Type of Compound Code(s): XA2400

Molecular Formula: C₁₂H₁₅N₅O₃

Molecular Weight: 277.282

Accurate Mass: 277.11749

Percentage Composition: C 51.98%; H 5.45%; N 25.26%; O 17.31%

Biological Use/Importance: Potent and selective inhibitor of hepatitis B virus

>>Variant: (1*R*,3*S*,4*R*)-form

CAS Registry Number: 188399-46-4

Molecular Formula: C₁₂H₁₅N₅O₃

Molecular Weight: 277.282

Accurate Mass: 277.11749

Percentage Composition: C 51.98%; H 5.45%; N 25.26%; O 17.31%

Optical Rotation: [α]_D -34.6 (c, 0.3 in H₂O) (>99% ee)

>>Variant: (1*S*,3*R*,4*S*)-form

CAS Registry Number: 142217-69-4

Molecular Formula: C₁₂H₁₅N₅O₃

Molecular Weight: 277.282

Accurate Mass: 277.11749

Percentage Composition: C 51.98%; H 5.45%; N 25.26%; O 17.31%

Physical Description: Cryst. (H₂O)

Optical Rotation: [α]_D +35 (c, 0.38 in H₂O) (>99% ee)

Other Data: Pharmacol. active isomer

References:

Eur. Pat., 1992, *Squibb*, 481 754; *CA*, **117**, 49162c, (*synth, pharmacol*)

Innaimo, S.F. *et al.*, *Antimicrob. Agents Chemother.*, 1997, **41**, 1444-1448; 1999, **43**, 190-193, (*pharmacol*)

Bisacchi, G.S. *et al.*, *Bioorg. Med. Chem. Lett.*, 1997, **7**, 127-132, (*synth, pharmacol*)