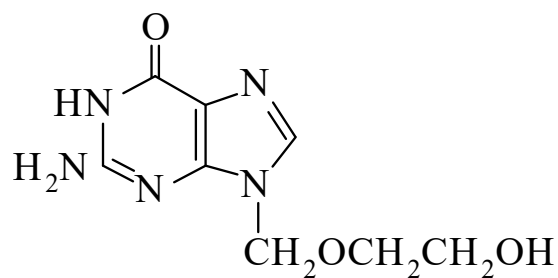




>>Entry Name: Aciclovir, BAN, INN, JAN

Synonym(s): 2-Amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]-6H-purin-6-one, 9Cl. 9-(2-Hydroxyethoxymethyl)guanine. Acyclovir, USAN. Acycloguanosine. Activir. Avirax. Cycloviran. Geavir. Herpetad. Milavir. Soothelip. Supraviran. Virasorb. Mirolex. Virovir. Zovirax. Zyclir. BW 248U. ACG



CAS Registry Number: 59277-89-3

Related CAS Registry Numbers(s): 124832-28-6 125581-72-8 142963-59-5 142963-60-8 142963-71-1

Molecular Formula: C<sub>8</sub>H<sub>11</sub>N<sub>5</sub>O<sub>3</sub>

Molecular Weight: 225.207

Accurate Mass: 225.08619

Percentage Composition: C 42.67%; H 4.92%; N 31.10%; O 21.31%

Biological Use/Importance: Antiviral agent

Physical Description: Cryst. (EtOH)

Development Status: Marketed drug. Worldwide 88th best selling prescription drug (\$0.57 bn) (GlaxoSmithKline) (2000, Pharma Business)

Melting Point: Mp 225° (dec.)

Calculated Log P Data: Log P -2.3 (calc)

Hazard & Toxicity: LD<sub>50</sub> (rat, ipr) 860 mg/kg. Exp. reprod. and teratogenic effects

Sigma: A4669

>>Derivative: Na salt

Synonym(s): Acyclovir sodium, USAN

CAS Registry Number: 69657-51-8

Hazard & Toxicity: LD<sub>50</sub> (rat, ipr) 1210 mg/kg. Exp. reprod. and teratogenic effects

>>Derivative: 6-Deoxy

Synonym(s): 2-[(2-Amino-9H-purin-9-yl)methoxy]ethanol. Desciclovir, INN, USAN. 6-Deoxyacyclovir. BWA 515U

CAS Registry Number: 84408-37-7

Molecular Formula: C<sub>8</sub>H<sub>11</sub>N<sub>5</sub>O<sub>2</sub>

Molecular Weight: 209.207

Accurate Mass: 209.091275

Percentage Composition: C 45.93%; H 5.30%; N 33.48%; O 15.30%

Biological Use/Importance: Antiviral agent (prodrug of Acyclovir)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 187-189°

Solubility: Sol. H<sub>2</sub>O

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

>>Derivative: 6-Deoxy, O-Ac

CAS Registry Number: 92924-35-1

Molecular Formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>

Molecular Weight: 251.244

Accurate Mass: 251.10184

Percentage Composition: C 47.81%; H 5.22%; N 27.87%; O 19.10%

Physical Description: Needles (EtOH)

Melting Point: Mp 135-136°