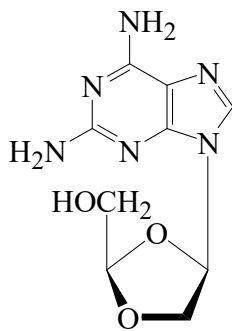




>>Entry Name: **2,6-Diamino-9-[2-(hydroxymethyl)-1,3-dioxolan-4-yl]purine**

Synonym(s): 4-(2,6-Diamino-9*H*-purin-9-yl)-1,3-dioxolane-2-methanol, 9Cl. DAPD



CAS Registry Number: 153611-19-9

Molecular Formula: C₉H₁₂N₆O₃

Molecular Weight: 252.232

Accurate Mass: 252.097089

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Biological Use/Importance: Anti-HIV agent

Other Data: Prodrug of 9-[2-(Hydroxymethyl)-1,3-dioxolan-4-yl]guanine [JHH61-R](#)

>>Variant: (2*R*,4*R*)-form

CAS Registry Number: 145514-04-1

Molecular Formula: C₉H₁₂N₆O₃

Molecular Weight: 252.232

Accurate Mass: 252.097089

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Physical Description: Microneedles (MeOH)

Melting Point: Mp 236-237°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -71.44$ (c, 0.25 in MeOH)

Other Data: Pharmacol. active isomer

>>Variant: (2*S*,4*R*)-form

CAS Registry Number: 147060-53-5

Molecular Formula: C₉H₁₂N₆O₃

Molecular Weight: 252.232

Accurate Mass: 252.097089

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Physical Description: Solid (Et₂O)

Melting Point: Mp 148-149°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -24.24$ (c, 0.26 in MeOH)

>>Variant: (2*S*,4*S*)-form

CAS Registry Number: 147060-52-4

Molecular Formula: C₉H₁₂N₆O₃

Molecular Weight: 252.232

Accurate Mass: 252.097089

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 176-178°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +29.4$ (c, 0.32 in MeOH)

References:

Kim, H.O. *et al.*, *J. Med. Chem.*, 1993, **36**, 30-37; 519-528, (*synth, pharmacol*)

Pat. Coop. Treaty (WIPO), 1994, *Emory Univ.*, 94 09 793; *CA*, **121**, 99776j, (*synth, isomers, pharmacol*)

Gu, Z. *et al.*, *Antimicrob. Agents Chemother.*, 1999, **43**, 2376-2382, (*activity*)