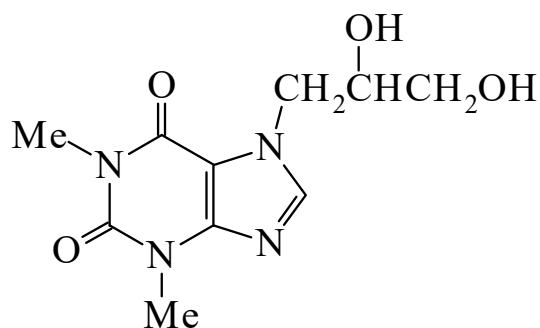




>>Entry Name: **Diprophylline**, BAN, INN

Synonym(s): 7-(2,3-Dihydroxypropyl)-3,7-dihydro-1,3-dimethyl-1*H*-purine-2,6-dione, 9Cl. 7-(2,3-Dihydroxypropyl)theophylline, 8Cl. Diprofilin. **Dyphylline**, USAN. Glyfyllin. Glyphylline. Hyphylline. Theocardin. Asthmolysin. Neophyllin. Neutraphylline. Many other names



CAS Registry Number: 479-18-5

Type of Compound Code(s): XA1100 XA1650 XA2250 XA3850

Molecular Formula: C₁₀H₁₄N₄O₄

Molecular Weight: 254.245

Accurate Mass: 254.101506

Percentage Composition: C 47.24%; H 5.55%; N 22.04%; O 25.17%

Biological Use/Importance: Antihypertensive agent, diuretic, spasmolytic and antiasthmatic drug

Calculated Log P Data: Log P –1.71 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 1954 mg/kg

Aldrich: D11940-7

Fluka: 37910

Sigma: D0633

>>Variant: (*R*)-form

CAS Registry Number: 72376-78-4

Molecular Formula: C₁₀H₁₄N₄O₄

Molecular Weight: 254.245

Accurate Mass: 254.101506

Percentage Composition: C 47.24%; H 5.55%; N 22.04%; O 25.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 159-160°

Optical Rotation: [α]_D²⁰+88.2 (c, 0.5 in H₂O)

>>Derivative: Di-Ac

Melting Point: Mp 125-126°

Optical Rotation: [α]_D²⁰+73.9 (c, 0.5 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 68350-70-9

Molecular Formula: C₁₀H₁₄N₄O₄

Molecular Weight: 254.245

Accurate Mass: 254.101506

Percentage Composition: C 47.24%; H 5.55%; N 22.04%; O 25.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 158°

>>Derivative: Bis nicotinate

see Diniprophylline, [BNV81-V](#)

References: