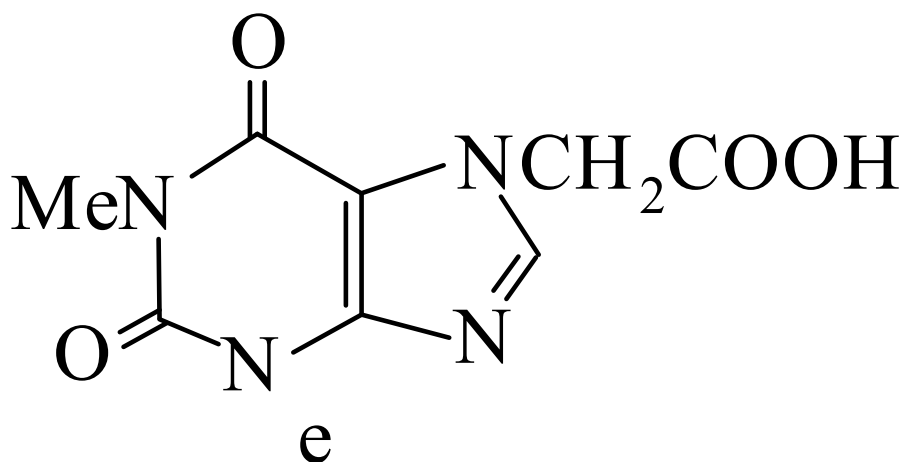




>>Entry Name: Acefylline

Synonym(s): 1,2,3,6-Tetrahydro-1,3-dimethyl-2,6-dioxo-7*H*-purine-7-acetic acid, 9Cl, 8Cl. 1,3-Dimethylxanthin-7-ylacetic acid. Theophylline-7-acetic acid. Aminodal. Stenofillina



CAS Registry Number: 652-37-9

Molecular Formula: C₉H₁₀N₄O₄

Molecular Weight: 238.202

Accurate Mass: 238.070206

Percentage Composition: C 45.38%; H 4.23%; N 23.52%; O 26.87%

Use/Importance: Spasmolytic, cardiotonic, diuretic and smooth muscle relaxant. Bronchodilator

Physical Description: Solid + 1H₂O

Melting Point: Mp 269-271°

Calculated Log P Data: Log P -0.65 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 2733 mg/kg

Fluka: 88310

Rare Chemicals Library: S41015-2

>>Derivative: Piperazine salt (2:1)

Synonym(s): Acefylline piperazine, INN. **Acepifylline**, BAN. Etophyllate. Etaphylline

CAS Registry Number: 18428-63-2

Molecular Formula: C₂₂H₃₀N₁₀O₈

Molecular Weight: 562.541

Accurate Mass: 562.22481

Percentage Composition: C 46.97%; H 5.38%; N 24.90%; O 22.75%