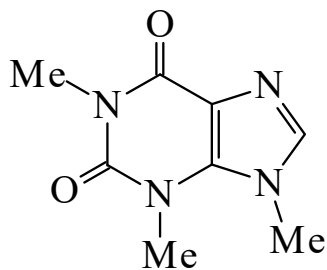




>>Entry Name: 1,3,9-Trimethyl-9*H*-purine-2,6(1*H*,3*H*)-dione

Synonym(s): 1,3,9-Trimethylisoxanthine. Isocaffeine



CAS Registry Number: 519-32-4

Molecular Formula: C₈H₁₀N₄O₂

Molecular Weight: 194.193

Accurate Mass: 194.080376

Percentage Composition: C 49.48%; H 5.19%; N 28.85%; O 16.48%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 294-295° (285-287°)

Other Data: Sublimes

Fluka: 92765

Sigma: T4146

References:

Blicke, F.F. *et al.*, *J.A.C.S.*, 1956, **78**, 5857

Chaman, E.S. *et al.*, *Zh. Obshch. Khim.*, 1960, **30**, 1873; *CA*, **55**, 8417

Ovcharova, I.M. *et al.*, *Zh. Obshch. Khim.*, 1962, **32**, 2010; *CA*, **58**, 4567, (*synth*)

Horváth, A. *et al.*, *Synthesis*, 1995, 1183, (*synth*)