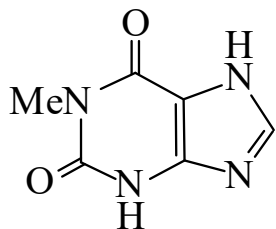




>>Entry Name: 3,7-Dihydro-1-methyl-1*H*-purine-2,6-dione, 9Cl

Synonym(s): 1-Methylxanthine



CAS Registry Number: 6136-37-4

Extra CAS Registry Numbers(s): 28109-92-4

Molecular Formula: C₆H₆N₄O₂

Molecular Weight: 166.139

Accurate Mass: 166.049076

Percentage Composition: C 43.38%; H 3.64%; N 33.72%; O 19.26%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 350°

Hazard & Toxicity: LD₅₀ (mus, ipr) 510 mg/kg

Aldrich: 28098-4

Fluka: 69720

Sigma: M3275

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 213B, (*nmr*)

Black, T.H. *et al.*, *Synth. Commun.*, 1989, **19**, 843