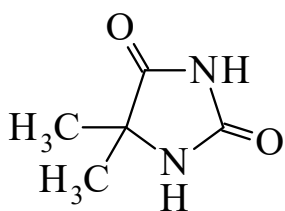




>>Entry Name: 5,5-Dimethyl-2,4-imidazolidinedione, 9CI

Synonym(s): 5,5-Dimethylhydantoin



CAS Registry Number: 77-71-4

Molecular Formula: C₅H₈N₂O₂

Molecular Weight: 128.13

Accurate Mass: 128.058578

Percentage Composition: C 46.87%; H 6.29%; N 21.86%; O 24.97%

Use/Importance: Reagent for amine synth.

Physical Description: Prisms (EtOH)

Melting Point: Mp 175°

Solubility: Sol. H₂O

pKa Value: pK_a 9.19 (24°)

Other Data: Sublimes

Aldrich: D16140-3

Fluka: 40670

Rare Chemicals Library: S4058-5

Sigma: D4504

>>Derivative: N³-Ac

Molecular Formula: C₇H₁₀N₂O₃

Molecular Weight: 170.168

Accurate Mass: 170.069143

Percentage Composition: C 49.41%; H 5.92%; N 16.46%; O 28.21%

Melting Point: Mp 192°

>>Derivative: N¹,N³-Di-Ac

CAS Registry Number: 36452-35-4

Molecular Formula: C₉H₁₂N₂O₄

Molecular Weight: 212.205

Accurate Mass: 212.079708

Percentage Composition: C 50.94%; H 5.70%; N 13.20%; O 30.16%

Melting Point: Mp 186-187°

>>Derivative: N¹-Me, N³-Ac

Synonym(s): 3-Acetyl-1,5,5-trimethyl-2,4-imidazolidinedione

CAS Registry Number: 22820-92-4

Molecular Formula: C₈H₁₂N₂O₃

Molecular Weight: 184.194

Accurate Mass: 184.084793

Percentage Composition: C 52.17%; H 6.57%; N 15.21%; O 26.06%

Use/Importance: Selective acetylating agent for phenolic OH groups

Melting Point: Mp 126-127°

>>Derivative: N¹-Me

Synonym(s): 1,5,5-Trimethyl-2,4-imidazolidinedione

Molecular Formula: C₆H₁₀N₂O₂

Molecular Weight: 142.157

Accurate Mass: 142.074228

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 162.5-163°