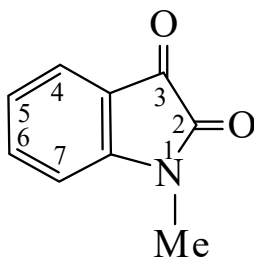




>>Entry Name: 1-Methyl-1*H*-indole-2,3-dione, 9CI

Synonym(s): 1-Methylisatin



CAS Registry Number: 2058-74-4

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Physical Description: Red-yellow needles (H₂O)

Melting Point: Mp 134°

Solubility: Sol. MeOH, hot H₂O; mod. sol. Et₂O

Other Data: Dimorphous (both forms orthorhombic). Stable in air

Hazard & Toxicity: LD₅₀ (mus, ipr) 685 mg/kg

Aldrich: 18307-5

>>Derivative: 2-Oxime

Molecular Formula: C₉H₈N₂O₂

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Physical Description: Needles (H₂O)

Melting Point: Mp 189-192°

>>Derivative: 2-Oxime, Ac

Molecular Formula: C₁₁H₁₀N₂O₃

Molecular Weight: 218.212

Accurate Mass: 218.069143

Percentage Composition: C 60.55%; H 4.62%; N 12.84%; O 22.00%

Physical Description: Yellow cryst.

Melting Point: Mp 154-155°

>>Derivative: 3-Hydrazone

Molecular Formula: C₉H₉N₃O

Molecular Weight: 175.19

Accurate Mass: 175.074562

Percentage Composition: C 61.70%; H 5.18%; N 23.99%; O 9.13%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 107-108°

>>Derivative: 3-Phenylhydrazone

Physical Description: Yellow needles (EtOH)

Solubility: Sol. hot EtOH, C₆H₆; spar. sol. Et₂O, insol. petrol

>>Derivative: 2-Anil

Molecular Formula: C₁₅H₁₂N₂O

Molecular Weight: 236.273

Accurate Mass: 236.094963

Percentage Composition: C 76.25%; H 5.12%; N 11.86%; O 6.77%

Physical Description: Yellowish-red prisms

Melting Point: Mp 132°

>>Derivative: 3-Thiosemicarbazone

Synonym(s): Methisazone, BAN, USAN. **Metisazone**, INN. Marboran. BW 33-T-57. NSC 69811