



>>Entry Name: 5-Methyl-1*H*-indole-2,3-dione, 9CI

Synonym(s): 5-Methylisatin

CAS Registry Number: 608-05-9

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 plates (H₂O), red needles (EtOH)

Melting Point: Mp 187°

Hazard & Toxicity: LD₅₀ (mus, ipr) 790 mg/kg

Rare Chemicals Library: S50960-4

Sigma: M3002

>>Derivative: 3-Oxime

CAS Registry Number: 13208-98-5

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%

Melting Point: Mp 222-224°

>>Derivative: 3-Phenylhydrazone

Melting Point: Mp 268°

>>Derivative: *N*-Ac

CAS Registry Number: 118726-65-1

Molecular Formula: C₁₁H₉NO₃

Molecular Weight: 203.197

Accurate Mass: 203.058244

Percentage Composition: C 65.02%; H 4.46%; N 6.89%; O 23.62%

Physical Description: Yellow needles

Melting Point: Mp 172°

Solubility: Spar. sol. H₂O, EtOH, Et₂O; sol. C₆H₆

>>Derivative: *N*-Benzoyl

CAS Registry Number: 99448-76-7

Molecular Formula: C₁₆H₁₁NO₃

Molecular Weight: 265.268

Accurate Mass: 265.073894

Percentage Composition: C 72.45%; H 4.18%; N 5.28%; O 18.09%

Physical Description: Yellow-green needles (C₆H₆)

Melting Point: Mp 193°

Solubility: Spar. sol. EtOH

>>Derivative: *N*-(4-Methylbenzenesulfonyl)

CAS Registry Number: 99448-78-9

Melting Point: Mp 202-205°

>>Derivative: *N*-Me

Synonym(s): 1,5-Dimethyl-1*H*-indole-2,3-dione, 9CI. 1,5-Dimethylisatin

CAS Registry Number: 66440-60-6

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Red needles

Melting Point: Mp 148°