



>>Entry Name: 5-Nitro-1*H*-indole-2,3-dione, 9Cl

Synonym(s): 5-Nitroisatin

CAS Registry Number: 611-09-6

Molecular Formula: C₈H₄N₂O₄

Molecular Weight: 192.131

Accurate Mass: 192.017108

Percentage Composition: C 50.01%; H 2.10%; N 14.58%; O 33.31%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 254-255 dec.°

Solubility: Sol. alkalis with red colour; spar. sol. H₂O

Aldrich: N1780-7

>>Derivative: *N*-Ac

Molecular Formula: C₁₀H₆N₂O₅

Molecular Weight: 234.168

Accurate Mass: 234.027673

Percentage Composition: C 51.29%; H 2.58%; N 11.96%; O 34.16%

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 193-194°

>>Derivative: 3-Oxime, benzyl ether

Molecular Formula: C₁₅H₁₁N₃O₄

Molecular Weight: 297.27

Accurate Mass: 297.074957

Percentage Composition: C 60.61%; H 3.73%; N 14.14%; O 21.53%

Melting Point: Mp 234-235°

Solubility: Sol. Me₂CO, C₆H₆; spar. sol. EtOH

>>Derivative: 3-Phenylhydrazone

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 295°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-5-nitro-1*H*-indole-2,3-dione

CAS Registry Number: 3484-32-0

Molecular Formula: C₉H₆N₂O₄

Molecular Weight: 206.157

Accurate Mass: 206.032758

Percentage Composition: C 52.44%; H 2.93%; N 13.59%; O 31.04%

Physical Description: Orange needles (AcOH aq.)

Melting Point: Mp 204-206°

>>Derivative: *N*-Me, hydrazone

Molecular Formula: C₉H₈N₄O₃

Molecular Weight: 220.187

Accurate Mass: 220.059641

Percentage Composition: C 49.09%; H 3.66%; N 25.45%; O 21.80%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 210 dec.°

References: