



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

Synonym(s): 5-Chloroisatin

CAS Registry Number: 17630-76-1

Structure by analogy with 4-Chloro-1*H*-indole-2,3-dione, [FVS96-K](#)

Molecular Formula: C₈H₄ClNO₂

Molecular Weight: 181.578

Accurate Mass: 180.993056

Percentage Composition: C 52.92%; H 2.22%; Cl 19.52%; N 7.71%; O 17.62%

Physical Description: Orange-yellow cryst.

Melting Point: Mp 247 dec.°

Solubility: Spar. sol. hot H₂O

Rare Chemicals Library: S56459-1

>>Derivative: 3-Oxime

CAS Registry Number: 85124-16-9

Molecular Formula: C₈H₅ClN₂O₂

Molecular Weight: 196.592

Accurate Mass: 196.003955

Percentage Composition: C 48.88%; H 2.56%; Cl 18.03%; N 14.25%; O 16.28%

Physical Description: Pale yellow cryst.

Melting Point: Mp 252°

>>Derivative: *N*-Chloro

Synonym(s): 1,5-Dichloro-1*H*-indole-2,3-dione. 1,5-Dichloroisatin

Molecular Formula: C₈H₃Cl₂NO₂

Molecular Weight: 216.023

Accurate Mass: 214.954083

Percentage Composition: C 44.48%; H 1.40%; Cl 32.82%; N 6.48%; O 14.81%

Physical Description: Red prisms (AcOH)

Melting Point: Mp 155°

>>Derivative: *N*-Me

CAS Registry Number: 60434-13-1

Molecular Formula: C₉H₆ClNO₂

Molecular Weight: 195.605

Accurate Mass: 195.008706

Percentage Composition: C 55.26%; H 3.09%; Cl 18.12%; N 7.16%; O 16.36%

Physical Description: Solid

Melting Point: Mp 171-173°

References:

- Buchman, E.R. *et al.*, *J.A.C.S.*, 1946, **68**, 2692-2695, (*N-chloro*)
Buu-Hoï, Ng.Ph., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1954, **73**, 197
Gassmann, P.G. *et al.*, *J.O.C.*, 1977, **42**, 1344-1348, (*synth*)
Kearney, T. *et al.*, *Synthesis*, 1992, 769-772, (*synth*)
Webber, S.E. *et al.*, *J. Med. Chem.*, 1996, **39**, 5072-5082, (*N-Me, synth, pmr, ir*)
Meth-Cohn, O. *et al.*, *Tet. Lett.*, 1996, **37**, 9381-9384, (*synth*)
Smith, K. *et al.*, *Synlett*, 1999, 945-947, (*synth*)