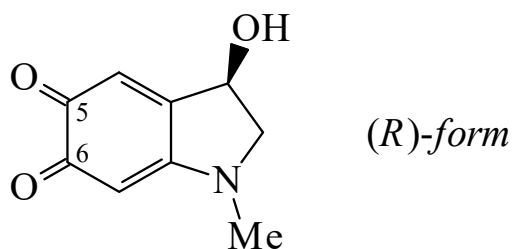




>>Entry Name: Adrenochrome

Synonym(s): 2,3-Dihydro-3-hydroxy-1-methyl-1*H*-indole-5,6-dione, 9Cl



CAS Registry Number: 54-06-8

Molecular Formula: C₉H₉NO₃

Molecular Weight: 179.175

Accurate Mass: 179.058244

Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%

Use/Importance: Has a variety of physiol. props. incl. hallucinogenic

Calculated Log P Data: Log P −1.49 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (rat, ipr) 150 mg/kg

Sigma: A5752

>>Variant: (*R*)-form

CAS Registry Number: 7506-92-5

Molecular Formula: C₉H₉NO₃

Molecular Weight: 179.175

Accurate Mass: 179.058244

Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%

Source/Synthesis: Obt. by oxidn. of adrenaline by various means

Physical Description: Unstable deep violet-red needles

Optical Rotation: $[\alpha]_{630}^{25} +150$

Other Data: Readily oxidised → melanin. Dec. between 100° and 135°

>>Variant: (±)-form

Molecular Formula: C₉H₉NO₃

Molecular Weight: 179.175

Accurate Mass: 179.058244

Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%

Physical Description: Reddish-violet rods

Melting Point: Mp 125° (dec.)

Solubility: V. sol. H₂O, EtOH

>>Derivative: *p*-Nitrophenylhydrazone

Physical Description: Brown needles + 4H₂O (dioxan)

Melting Point: Mp 200°

>>Derivative: 5-Semicarbazone

Synonym(s): 2-(1,2,3,6-Tetrahydro-3-hydroxy-1-methyl-6-oxo-5*H*-indol-5-ylidene)hydrazinecarboxamide, 9Cl. **Carbazochrome**, INN, JAN. Adrenosem. Adrenoxyl. Adrestat F

CAS Registry Number: 69-81-8

Molecular Formula: C₁₀H₁₂N₄O₃

Molecular Weight: 236.23

Accurate Mass: 236.090941

Percentage Composition: C 50.84%; H 5.12%; N 23.72%; O 20.32%

Use/Importance: Antihæmorrhagic

Melting Point: Mp 202-204°. Mp 212-213° (dec.)

Sigma: A5877