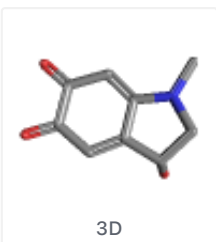
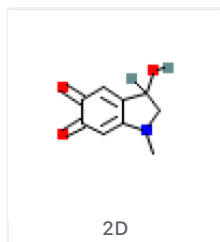


Adrenochrome

[Cite](#)[Download](#)**PubChem CID**

5898

Structure[Find Similar Structures](#)**Molecular Formula**C9H9NO3**Synonyms**

Adrenochrome

54-06-8

Adraxone

3-Hydroxy-1-methylindoline-5,6-dione

3-Hydroxy-1-methyl-5,6-indolinedione

[More...](#)**Molecular Weight**

179.17

Dates

Modify

Create

2021-12-18

2005-03-26

Description

Adrenochrome is a member of indoles.

[► ChEBI](#)

Pigment obtained by the oxidation of epinephrine.

▶ [Medical Subject Headings \(MeSH\)](#)

Contents



1 Structures



2 Names and Identifiers



3 Chemical and Physical Properties



4 Spectral Information



5 Related Records



6 Chemical Vendors

7 Toxicity



8 Literature



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10 Biological Test Results



11 Classification



12 Information Sources

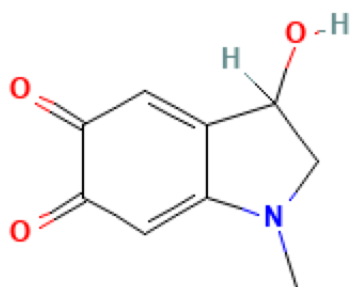
1 Structures



1.1 2D Structure



Chemical Structure Depiction



► [PubChem](#)

1.2 3D Conformer



► [PubChem](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



3-hydroxy-1-methyl-2,3-dihydroindole-5,6-dione

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

[▶ PubChem](#)

2.1.2 InChI



InChI=1S/C9H9NO3/c1-10-4-9(13)5-2-7(11)8(12)3-6(5)10/h2-3,9,13H,4H2,1H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

[▶ PubChem](#)

2.1.3 InChI Key



RPHLQSHHTJORHI-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

[▶ PubChem](#)

2.1.4 Canonical SMILES



CN1CC(C2=CC(=O)C(=O)C=C2)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

[▶ PubChem](#)

2.2 Molecular Formula



C9H9NO3

Computed by PubChem 2.1 (PubChem release 2021.05.07)

[▶ PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



54-06-8

- ▶ [CAS Common Chemistry; ChemIDplus; European Chemicals Agency \(ECHA\)](#)

7506-92-5

- ▶ [DTP/NCI](#)

2.3.2 European Community (EC) Number



200-192-8

- ▶ [European Chemicals Agency \(ECHA\)](#)

2.3.3 NSC Number



383491

- ▶ [DTP/NCI](#)

407840

- ▶ [DTP/NCI](#)

2.3.4 Wikipedia



Adrenochrome

- ▶ [Wikipedia](#)

2.4 Synonyms



2.4.1 MeSH Entry Terms



Adrenochrome

- ▶ [Medical Subject Headings \(MeSH\)](#)

2.4.2 Depositor-Supplied Synonyms



Adrenochrome	EINECS 200-192-8	AKOS00
54-06-8	Adrenochrom	NSC-3E
Adraxone	D,L-Adrenochrome	NSC-4C
3-Hydroxy-1-methylindoline-5,6-dione	2,3-Dihydro-3-hydroxy-1-methyl-1H-indole-5,6-dione	NCGC0
3-Hydroxy-1-methyl-5,6-indolinedione	adrenochrome free base	FT-062
1-Adrenochrome	Adrenochrome, free base	A-3200
5,6-INDOLINEDIONE, 3-HYDROXY-1-METHYL-	ADRENOCHROME, L-	Q36680
3-hydroxy-1-methyl-2,3-dihydroindole-5,6-dione	SCHEMBL61927	3-hydr
MFCD00069732	CHEMBL1314174	1H-Ind
NSC407840	DTXSID00871530	7506-9
3-hydroxy-1-methyl-2,3-dihydro-1H-indole-5,6-dione	CHEBI:166544	D,L-Adr
3-Hydroxy-1-methyl-5,6-indolinedione, 98%	BCP30577	pound>
USAF uctI-7	NSC383491	

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	179.17	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	-1.3	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	179.058243149	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	179.058243149	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	57.6 Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	13	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	354	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	1	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

► [PubChem](#)

4 Spectral Information



4.1 1D NMR Spectra



4.1.1 ¹³C NMR Spectra



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Thumbnail

► [SpectraBase](#)

5 Related Records



5.1 Related Compounds with Annotation



▶ PubChem

5.2 Related Compounds



Same Connectivity 3 Records
Same Parent, Connectivity 5 Records
Same Parent, Exact 3 Records
Mixtures, Components, and Neutralized Forms 9 Records
Similar Compounds 10 Records
Similar Conformers 549 Records

▶ PubChem

5.3 Substances



5.3.1 Related Substances



All 79 Records
Same 68 Records

Mixture

11 Records

▶ PubChem

5.3.2 Substances by Category



▶ PubChem

▶ PubChem

7 Toxicity



7.1 Toxicological Information



7.1.1 Acute Effects



► [ChemIDplus](#)

8 Literature



8.1 NLM Curated PubMed Citations



▶ PubChem

8.2 Springer Nature References



▶ Springer Nature

8.3 Thieme References



▶ Thieme Chemistry

8.4 Chemical Co-Occurrences in Literature



▶ PubChem

8.5 Chemical-Gene Co-Occurrences in Literature



▶ PubChem

8.6 Chemical-Disease Co-Occurrences in Literature



► PubChem

9 Patents



9.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

9.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=RPHLQSHHTJORHI-UHFFFAOYSA-N>

▶ PATENTSCOPE (WIPO)

10 Biological Test Results



10.1 BioAssay Results



▶ [PubChem](#)

11 Classification



11.1 Ontologies



11.1.1 MeSH Tree



▶ Medical Subject Headings (MeSH)

11.1.2 ChEBI Ontology



▶ ChEBI

11.1.3 ChemIDplus



▶ ChemIDplus

11.1.4 NORMAN Suspect List Exchange Classification



▶ NORMAN Suspect List Exchange

12 Information Sources



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1. CAS Common Chemistry

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Adrenochrome

https://commonchemistry.cas.org/detail?cas_rn=54-06-8

2. ChemIDplus

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Adrenochrome

<https://chem.nlm.nih.gov/chemidplus/sid/0000054068>

ChemIDplus Chemical Information Classification

<https://chem.nlm.nih.gov/chemidplus/>

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<https://echa.europa.eu/web/guest/legal-notice>

3-hydroxy-1-methylindoline-5,6-dione

<https://echa.europa.eu/substance-information/-/substanceinfo/100.000.176>

5. ChEBI

Adrenochrome

<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:166544>

ChEBI Ontology

<http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology>

6. **SpectraBase**

ADRENOCHROME

<https://spectrabase.com/spectrum/FmM6Dhu2g30>

7. **Springer Nature**

<https://pubchem.ncbi.nlm.nih.gov/substance/341140828>

8. **Thieme Chemistry**

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9. **Wikipedia**

adrenochrome

<https://en.wikipedia.org/wiki/Adrenochrome>

10. **Medical Subject Headings (MeSH)**

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Adrenochrome

<https://www.ncbi.nlm.nih.gov/mesh/68000323>

MeSH Tree

<http://www.nlm.nih.gov/mesh/meshhome.html>

11. **PubChem**

<https://pubchem.ncbi.nlm.nih.gov>

12. **NORMAN Suspect List Exchange**

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NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

13. **PATENTSCOPE (WIPO)**

SID 389187508

<https://pubchem.ncbi.nlm.nih.gov/substance/389187508>