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Lysergic Acid - Compound Summary (CID 622688)

Also known as: Isolysergic acid, 6-Methyl-9,10-didehydroergoline-8-carboxylic acid, D-Lysergic acid, (+)-Lysergic acid, AC1LDO0Z, L000805

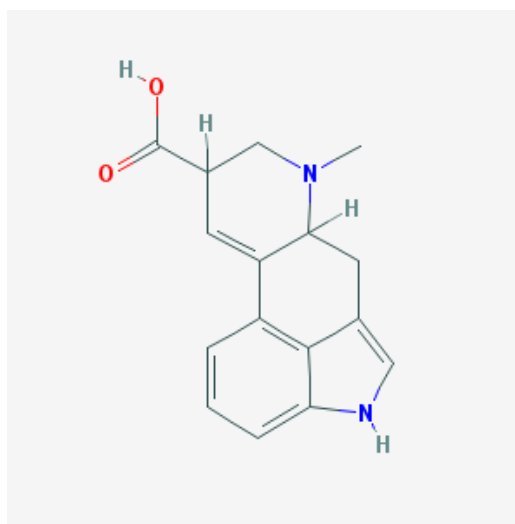
Molecular Formula: C₁₆H₁₆N₂O₂ **Molecular Weight:** 268.31044 **InChIKey:** ZAGRKAFMISFKIO-UHFFFAOYSA-N

Table of Contents

[Show subcontent titles](#)

[Identification](#)
[Related Records](#)
[Biomedical Effects and Toxicity](#)
[Literature](#)
[Biological Test Results](#)
[Classification](#)
[Chemical and Physical Properties](#)

[2D Structure](#) [3D Conformer](#)


[» Links and Relations](#)

Properties

Compound ID: 622688

Molecular Weight: 268.31

Molecular Formula: C₁₆H₁₆

XLogP3: 0

H-Bond Donor: 2

H-Bond Acceptor: 3

BioActivity Data

[This Compound with Similar Compounds](#)
[with Similar Conformers](#)

Related Compounds

[Same, Connectivity \(5\)](#)
[Similar Compounds \(239\)](#)
[Similar Conformers \(351\)](#)

Related Substances

[All \(14\)](#)
[Same Structure \(13\)](#)
[Mixture \(1\)](#)

Other Links

[PubMed \(2\)](#)
[NLM Toxicology Link](#)
[Chemical Structure Search](#)

Chemical Vendor

[ABI Chem](#)
[SID 109847548 - External](#)
[Chemical Synthesis Data](#)
[SID 126539490 - External](#)

Identification

Depositor-Supplied Synonyms

[Isolysergic acid](#)
[LYSERGIC ACID](#)
[6-Methyl-9,10-didehydroergoline-8-carboxylic acid](#)
[D-Lysergic acid](#)
[\(+\)-Lysergic acid](#)
[AC1LDO0Z](#)
[L000805](#)
[\(8alpha\)-9,10-Didehydro-6-methylergoline-8-carboxylic acid](#)
[Ergoline-8-carboxylic acid, 9,10-didehydro-6-methyl-, \(8.beta.\)-](#)
[Ergoline-8-carboxylic acid, 9,10-didehydro-6-methyl-, \(8alpha\)-](#)

... see all 12

Compound Information

CID 622688

Create Date: 2005-03-28

Descriptors

IUPAC Name: 7-methyl-6,6a,8,9-tetrahydro-4H-indolo[4,3-fg]quinoline-9-carboxylic acid

InChI: InChI=1S/C16H16N2O2/c1-18-8-10(16(19)20)5-12-11-3-2-4-13-15(11)9(7-17-13)6-14(12)18/h2-5,7,10,14,17H,6,8H2,1H3,(H,19,20)

InChIKey: ZAGRKAFMISFKIO-UHFFFAOYSA-N

Canonical SMILES : CN1CC(C=C2C1CC3=CNC4=CC=CC2=C34)C(=O)O

Related Records

Related Compounds

Same, Connectivity: [5 records](#)
 Similar Compounds: [239 records](#)
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[show all 2 sub-sections \(Related Compounds, Related Substances\)](#)

Biomedical Effects and Toxicity

Toxicology References

[ClinicalTrials.gov](#) - clinical trials

[DART](#) - Developmental and Reproductive Toxicology and Environmental Teratology Information Center - Current and older literature on developmental and reproductive toxicology.

[TOXLINE](#) - biochemical, pharmacological, physiological, and toxicological effects of drugs and other chemicals.

from [ChemIDplus](#)

Literature

Depositor Provided PubMed Citations

PubMed: [2 records](#)

[show all 2 sub-sections \(Depositor Provided PubMed Citations, NLM Curated PubMed Citations\)](#)

Biological Test Results

BioAssay Results

#	AID	SID	Activity		BioAssay	BioAssay Type	Protein Target	DataTable Reference
			Outcome Type	Value [μ M]				
1	2062	85209518	■		Ligands of bioamine (Class A) GPCRs	other		
2	624193	135650563	■		Agonists at Mouse 5-Hydroxytryptamine receptor 5-ht5a	other	Htr5a gene product [Mus musculus] [gi:84370345]	
3	624199	135650563	■		Agonists at Human 5-Hydroxytryptamine receptor 5-HT1D	other	HTR1D gene product [Homo sapiens] [gi:4504535]	

Tested in BioAssays: All: [3](#) Active: [3](#)

BioActivity Summary:

[This Compound](#) with Similar Compounds with Similar Conformers

from [BioAssay](#)

Classification

MeSH (Medical Subject Headings) is the NLM controlled vocabulary thesaurus used for indexing articles for PubMed.

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[Alkaloids](#)
[Ergot Alkaloids](#)
[Ergolines](#)

[Lysergic Acid](#) ▾
[Heterocyclic Compounds with 4 or More Rings](#) ▾
[Ergolines](#) ▾
[Lysergic Acid](#) ▾

from MeSH

[show all 2 sub-sections \(Ontologies, Substance Categorization Classification\)](#)

Chemical and Physical Properties

Computed Properties

Molecular Weight	268.31044 [g/mol]
Molecular Formula	C ₁₆ H ₁₆ N ₂ O ₂
XLogP3	0
H-Bond Donor	2
H-Bond Acceptor	3
Rotatable Bond Count	1
Tautomer Count	2
Exact Mass	268.121178
Monoisotopic Mass	268.121178
Topological Polar Surface Area	56.3
Heavy Atom Count	20
Formal Charge	0
Complexity	461
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	2
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	1
Feature 3D Acceptor Count	2
Feature 3D Donor Count	1
Feature 3D Anion Count	1
Feature 3D Cation Count	2
Feature 3D Ring Count	4
Effective Rotor Count	1.8
Conformer Sampling RMSD	0.6
CID Conformer Count	10

You are here: [NCBI](#) > [Chemicals & Bioassays](#) > [PubChem](#) > [Compound Summary](#)

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