Lysergic Acid - Compound Summary (CID 622688)

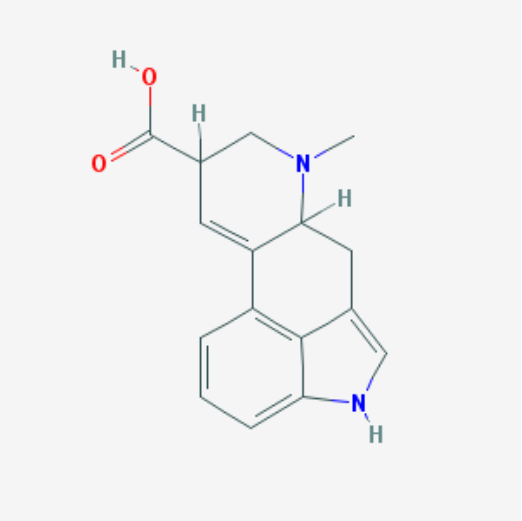
Also known as: Isolysergic acid, 6-Methyl-9,10-didehydroergoline-8-carboxylic acid, D-Lysergic acid, (+)-Lysergic acid, AC1LDO0Z, L000805

Molecular Formula: $C_{16}H_{16}N_2O_2$ **Molecular Weight:** 268.31044 **InChIKey:** ZAGRKAFMISFKIO-UHFFFAOYSA-N

Table of Contents Show subcontent titles

Expand all sub-sections

2D Structure 3D Conformer



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

» Links and Relat

Properties
Compound ID: 622688
Molecular Weight: 268.31
Molecular Formula: $C_{16}H$
XLogP3: 0
H-Bond Donor: 2
H-Bond Acceptor: 3

BioActivity Data
This Compound
with Similar Compounds
with Similar Conformers

Related Compou
Same, Connectivity (5)
Similar Compounds (239)
Similar Conformers (351)

Related Substanc
All (14)
Same Structure (13)
Mixture (1)

Other Links
PubMed (2)
NLM Toxicology Link
Chemical Structure Searc

Chemical Vendor
ABI Chem
SID 109847548 - Exte
Chemical Synthesis Data
SID 126539490 - Exte

Related Records

Related Compounds

Same, Connectivity: 5 records
Similar Compounds: 239 records
Similar Conformers: 351 records View Conformers

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 Outcome	Activity Type	Activity Value [µM]	BioAssay	BioAssay Type	Protein Target	DataTable Reference
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.

Heterocyclic Compounds
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	$C_{16}H_{16}N_2O_2$
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