Compound Summary for CID 5825

Dextroamphetamine Sulfate

Cite this Record

STRUCTURE VENDORS PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	5825
Chemical Names:	Ditab; Medex; D-Amphetamine sulphate; Amphetasul; Betafedrina; Betafedrine More...
Molecular Formula:	$C_{18}H_{28}N_2O_4S$
Molecular Weight:	368.492 g/mol
InChI Key:	PYHRZPFZZDCOPH-QXGOIDDHSA-N
Substance Registry:	FDA UNII
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)

Dextroamphetamine sulfate is the d-form of AMPHETAMINE. It is a central nervous system stimulant and a sympathomimetic. It has also been used in the treatment of narcolepsy and of attention deficit disorders and hyperactivity in children. Dextroamphetamine has multiple mechanisms of action including blocking uptake of adrenergics and dopamine, stimulating release of monamines, and inhibiting monoamine oxidase. It is also a drug of abuse and a psychotomimetic.

from MeSH

Dextroamphetamine Sulfate is the salt of the dextro-isomer of amphetamine and sympathomimetic amine with CNS stimulating properties. Dextroamphetamine sulphate acts by facilitating the release of catecholamines, particularly noradrenaline and dopamine, from nerve terminals in the brain and inhibits their uptake. This leads to an increase in motor activity, causes euphoria, mental alertness and excitement and suppresses appetite. This drug causes dependence and may cause an increase in heart rate and blood pressure. It is used in the treatment of narcolepsy and attention deficit hyperactivity disorder.

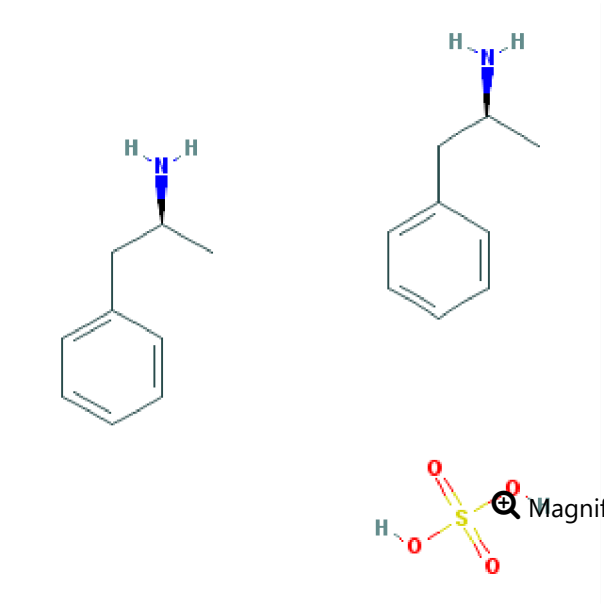
Pharmacology from NCIt

PUBCHEM > COMPOUND > DEXTROAMPHETAMINE SULFATE *Modify Date: 2018-09-15; Create Date: 2005-06-24*

Contents

1 2D Structure

Search Download Get Image



from PubChem

2 3D Status

Conformer generation is disallowed since mixture or salt

from PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(2S)-1-phenylpropan-2-amine;sulfuric acid

from PubChem

3.1.2 InChI

InChI=1S/2C9H13N.H2O4S/c2*1-8(10)7-9-5-3-2-4-6-9;1-5(2,3)4/h2*2-6,8H,7,10H2,1H3;(H2,1,2,3,4)/t2*8-;/m00./s1

from PubChem

3.1.3 InChI Key

PYHRZPFZZDCOPH-QXGOIDDHSA-N

from PubChem

3.1.4 Canonical SMILES

CC(CC1=CC=CC=C1)N.CC(CC1=CC=CC=C1)N.OS(=O)(=O)O

from PubChem

3.1.5 Isomeric SMILES

C[C@@H](CC1=CC=CC=C1)N.C[C@@H](CC1=CC=CC=C1)N.OS(=O)(=O)O

from PubChem

3.2 Molecular Formula

$C_{18}H_{28}N_2O_4S$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

51-63-8

from ChemIDplus, European Chemicals Agency (ECHA), The National Institute for Occupational Safety and Healt...

3.3.2 EC Number

200-111-6

from European Chemicals Agency (ECHA)

3.3.3 RTECS Number

SI1400000

from The National Institute for Occupational Safety and Health (NIOSH)

3.3.4 UNII

JJ768O327N

from FDA/SPL Indexing Data

3.3.5 Wikipedia

Title	(S)-amphetamine sulfate
Description	chemical compound

from Wikipedia

3.4 Synonyms

3.4.1 MeSH Entry Terms

1. Curban
2. d Amphetamine
3. d Amphetamine Sulfate
4. d-Amphetamine
5. d-Amphetamine Sulfate
6. Dexamfetamine
7. Dexamphetamine
8. Dexedrine
9. dextro Amphetamine
10. Dextro Amphetamine Sulfate
11. dextro-Amphetamine
12. Dextro-Amphetamine Sulfate
13. Dextroamphetamine
14. Dextroamphetamine Sulfate
15. DextroStat
16. Oxydess
17. Sulfate, Dextroamphetamine

from MeSH

3.4.2 Depositor-Supplied Synonyms

1. Ditab
2. Medex
3. d-Amphetamine sulphate
4. Amphetasul
5. Betafedrina
6. Betafedrine
7. Betaphedrine
8. Dellipsoids
9. Dextrosule
10. Dynaphenyl
11. Psychodrine
12. Tuphetamine
13. Acedron
14. Adjudets
15. Adrizine
16. Albemap
17. Amphaetex
18. Ampherex
19. Amptrerex
20. Apetain
21. Carrtime
22. Dexaline
23. Dexalme
24. Dexalone
25. Dexamed
26. Dexamine
27. Dexedrina
28. Dextenal
29. Diocurb
30. Diphylets
31. Domafate
32. Ephadren
33. Evrodex
34. Fastballs
35. Hetamine
36. Lentanet
37. Lipsoids
38. Lowedex
39. Obesedrin
40. Obesonil
41. Oranges
42. Pellcap
43. Phetadex
44. Pomadex
45. Recordati
46. Revidex
47. Spancap
48. Tempodex
49. Afatin
50. Amphex

from PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value
Molecular Weight	368.492 g/mol
Hydrogen Bond Donor Count	4
Hydrogen Bond Acceptor Count	6
Rotatable Bond Count	4
Complexity	166
CACTVS Substructure Key Fingerprint	AAADceB7OABAAAAAAAAAAAAAAAAAAAAAAAwYAAA AAAAAAABQAAAHAAQCAAADCjBGAQyAIBAAICAAiBCAD ACAAAgAAAIiIAAAIgIICKAkRGAIAAgkAAIiAcQgIAOAAAA AAAAAAAAAAAAAAAAAAAAAAAAAA==
Topological Polar Surface Area	135 A^2
Monoisotopic Mass	368.177 g/mol
Exact Mass	368.177 g/mol
Compound Is Canonicalized	true
Formal Charge	0
Heavy Atom Count	25
Defined Atom Stereocenter Count	2
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Isotope Atom Count	0
Covalently-Bonded Unit Count	3

from PubChem

4.2 Spectral Properties

4.2.1 Infrared Spectra

Infrared Spectra: 1 of 1 (ATR-IR Spectra)	
Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research

Infrared Spectra: 1 of 1 (ATR-IR Spectra)	
Source of Sample	Lipomed AG
Catalog Number	AMP-96-SU-50
Lot Number	96.1B6.1
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	CLICK TO LOAD...

from SpectraBase

4.2.2 Other Spectra

Other Spectra: 1 of 1 (Raman Spectra)	
Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Lipomed AG
Catalog Number	AMP-96-SU-50
Lot Number	96.1B6.1
Copyright	Copyright © 2013-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	CLICK TO LOAD...

from SpectraBase

5 Related Records

CLICK TO LOAD...

from NCBI

5.1 Related Compounds with Annotation

CLICK TO LOAD...

from PubChem

5.2 Related Compounds

Same Connectivity	5 records
Same Stereo	2 records
Same Isotope	3 records
Mixtures, Components, and Neutralized Forms	2 records
Similar Compounds	94 records

from PubChem

5.3 Substances

5.3.1 Related Substances

Same	32 records

from PubChem

5.3.2 Substances by Category

CLICK TO LOAD...

from PubChem

5.4 Entrez Crosslinks

Gene	3 records

from PubChem

6 Chemical Vendors

CLICK TO LOAD...

from PubChem

7 Pharmacology and Biochemistry

7.1 Pharmacology

Dextroamphetamine Sulfate is the salt of the dextro-isomer of amphetamine and sympathomimetic amine with CNS stimulating properties. Dextroamphetamine sulphate acts by facilitating the release of catecholamines, particularly noradrenaline and dopamine, from nerve terminals in the brain and inhibits their uptake. This leads to an increase in motor activity, causes euphoria, mental alertness and excitement and suppresses appetite. This drug causes dependence and may cause an increase in heart rate and blood pressure. It is used in the treatment of narcolepsy and attention deficit hyperactivity disorder.

from NCIt

7.2 MeSH Pharmacological Classification

Central Nervous System Stimulants

A loosely defined group of drugs that tend to increase behavioral alertness, agitation, or excitation. They work by a variety of mechanisms, but usually not by direct excitation of neurons. The many drugs that have such actions as side effects to their main therapeutic use are not included here.
See a list of PubChem compounds matching this category.

from MeSH

Dopamine Uptake Inhibitors

Drugs that block the transport of DOPAMINE into axon terminals or into storage vesicles within terminals. Most of the ADRENERGIC UPTAKE INHIBITORS also inhibit dopamine uptake.
See a list of PubChem compounds matching this category.

from MeSH

8 Safety and Hazards

8.1 Hazards Identification

8.1.1 GHS Classification

Signal: Danger
GHS Hazard Statements
Aggregated GHS information provided by 30 companies from 4 notifications to the ECHA C&L Inventory.

H300 (96.67%): Fatal if swallowed [Danger Acute toxicity, oral]

Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.

Precautionary Statement Codes
P264, P270, P301+P310, P321, P330, P405, and P501
(The corresponding statement to each P-code can be found here.)

from European Chemicals Agency (ECHA)

9 Toxicity

9.1 Toxicological Information

9.1.1 NIOSH Toxicity Data

Download

1 to 5 of 128 View More

Measurement	System	Route/Organism	Dose	Effect	Date
Reproductive Effects		intraperitoneal/rat	70 mg/kg (9-10D pregnant)	Reproductive: Effects on fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants)	July 2015
Reproductive Effects		intraperitoneal/mouse	500 µg/kg (8D pregnant)	Reproductive: Specific developmental abnormalities: Eye, ear Reproductive: Specific developmental abnormalities: Craniofacial (including nose and tongue) Reproductive: Specific developmental abnormalities: Cardiovascular (circulatory) system	July 2015
Reproductive Effects		intraperitoneal/mouse	500 µg/kg (8D pregnant)	Reproductive: Effects on fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants)	July 2015
Reproductive Effects		intraperitoneal/mouse	30 mg/kg (16-21D pregnant)	Reproductive: Effects on newborn: Biochemical and metabolic Reproductive: Effects on newborn: Behavioral	July 2015
Reproductive Effects		intraperitoneal/mouse	100 mg/kg (10D pregnant)	Reproductive: Effects on fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants) Reproductive: Specific developmental abnormalities: Central nervous system Reproductive: Specific developmental abnormalities: Musculoskeletal system	July 2015

from The National Institute for Occupational Safety and Health (NIOSH)

10 Literature

10.1 NLM Curated PubMed Citations

CLICK TO LOAD...

from PubChem

10.2 Springer Nature References

CLICK TO LOAD...

from Springer Nature

10.3 Chemical Co-Occurrences in Literature

CLICK TO LOAD...

View More Chemical-Chemical Co-Occurrences and Evidence for Dextroamphetamine Sulfate

from PubChem

10.4 Chemical-Disease Co-Occurrences in Literature

CLICK TO LOAD...

View More Chemical-Disease Co-Occurrences and Evidence for Dextroamphetamine Sulfate

from PubChem

10.5 Chemical-Gene Co-Occurrences in Literature

CLICK TO LOAD...

View More Chemical-Gene Co-Occurrences and Evidence for Dextroamphetamine Sulfate

from PubChem

11 Patents

11.1 Depositor-Supplied Patent Identifiers

CLICK TO LOAD...

from PubChem

12 Biological Test Results

12.1 BioAssay Results

CLICK TO LOAD...

from PubChem

13 Classification

13.1 Ontologies

13.1.1 MeSH Tree

CLICK TO LOAD...

from MeSH

13.1.2 KEGG: USP

CLICK TO LOAD...

from KEGG

13.1.3 KEGG: ATC

CLICK TO LOAD...

from KEGG

13.1.4 KEGG: Target-based Classification of Drugs

CLICK TO LOAD...

from KEGG

13.1.5 KEGG: Drug Classes

CLICK TO LOAD...

from KEGG

13.1.6 WHO ATC Classification System

CLICK TO LOAD...

from WHO ATC

13.1.7 WIPO IPC

CLICK TO LOAD...

from WIPO

13.1.8 ChemIDplus

CLICK TO LOAD...

from ChemIDplus

14 Information Sources

1. ## ChemIDplus /source/ChemIDplus
   Dextroamphetamine sulfate [USP]
   https://chem.nlm.nih.gov/chemidplus/sid/0000051638 https://chem.nlm.nih.gov/chemidplus/sid/0000051638
   ChemIDplus Chemical Information Classification
   https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp

2. ## European Chemicals Agency (ECHA) /source/European Chemicals Agency (ECHA)
   dexamphetamine sulphate
   https://echa.europa.eu/substance-information/-/substanceinfo/100.000.102 https://echa.europa.eu/substance-information/-/substanceinfo/100.000.102
   Dexamphetamine sulphate
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/69488 https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/69488

3. ## The National Institute for Occupational Safety and Health (NIOSH) /source/The National Institute for Occupational Safety and Health (NIOSH)
   Phenethylamine, alpha-methyl-, sulfate (2:1), (+)-
   https://www.cdc.gov/niosh-rtecs/SI155CC0.html https://www.cdc.gov/niosh-rtecs/SI155CC0.html

4. ## FDA/SPL Indexing Data /source/FDA/SPL Indexing Data
   JJ768O327N
   https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/ https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

5. ## NCIt /source/NCIt
   Dextroamphetamine Sulfate
   https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C47482 https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C47482

6. ## SpectraBase /source/SpectraBase
   https://spectrabase.com/spectrum/7D6JPTNeyzT https://spectrabase.com/spectrum/7D6JPTNeyzT
   https://spectrabase.com/spectrum/HOkCZdN6l44 https://spectrabase.com/spectrum/HOkCZdN6l44

7. ## Springer Nature /source/Springer Nature
   Literature references related to scientific contents from Springer Nature journals and books. Read more ... https://link.springer.com/

8. ## Wikipedia /source/Wikipedia
   (S)-amphetamine sulfate
   https://www.wikidata.org/wiki/Q27122300 https://www.wikidata.org/wiki/Q27122300

9. ## PubChem
   Data deposited in or computed by PubChem
   https://pubchem.ncbi.nlm.nih.gov https://pubchem.ncbi.nlm.nih.gov

10. ## MeSH /source/MeSH
    Dextroamphetamine
    https://www.ncbi.nlm.nih.gov/mesh/68003913 https://www.ncbi.nlm.nih.gov/mesh/68003913
    MeSH Tree
    http://www.nlm.nih.gov/mesh/meshhome.html http://www.nlm.nih.gov/mesh/meshhome.html
    Central Nervous System Stimulants
    https://www.ncbi.nlm.nih.gov/mesh/68000697 https://www.ncbi.nlm.nih.gov/mesh/68000697
    Dopamine Uptake Inhibitors
    https://www.ncbi.nlm.nih.gov/mesh/68018765 https://www.ncbi.nlm.nih.gov/mesh/68018765

11. KEGG /source/KEGG

USP drug classification
http://www.genome.jp/kegg-bin/get_htext?br08302.keg http://www.genome.jp/kegg-bin/get_htext?br08302.keg
Anatomical Therapeutic Chemical (ATC) classification
http://www.genome.jp/kegg-bin/get_htext?br08303.keg http://www.genome.jp/kegg-bin/get_htext?br08303.keg
Target-based classification of drugs
http://www.genome.jp/kegg-bin/get_htext?br08310.keg http://www.genome.jp/kegg-bin/get_htext?br08310.keg
Drug Classes
http://www.genome.jp/kegg-bin/get_htext?br08330.keg http://www.genome.jp/kegg-bin/get_htext?br08330.keg

12. WIPO /source/WIPO

International Patent Classification
http://www.wipo.int/classifications/ipc/ http://www.wipo.int/classifications/ipc/

13. WHO ATC /source/WHO ATC

ATC Code
https://www.whocc.no/atc_ddd_index/ https://www.whocc.no/atc_ddd_index/

14. NCBI

LinkOut is a service that allows one to link directly from NCBI databases to a wide range of information and services beyond NCBI systems.
https://www.ncbi.nlm.nih.gov/projects/linkout https://www.ncbi.nlm.nih.gov/projects/linkout