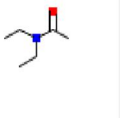
PubChem

COMPOUND SUMMARY

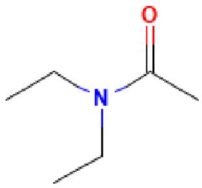
N,N-Diethylacetamide

PubChem CID	12703
Structure	 2D  3D Find Similar Structures
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_6H_{13}NO$
Synonyms	N,N-DIETHYLACETAMIDE 685-91-6 Acetamide, N,N-diethyl- N-Acetyldiethylamine UNII-6YO81D7ST6 More...
Molecular Weight	115.17
Dates	Modify 2021-09-11 Create 2005-03-26

1 Structures

1.1 2D Structure

Chemical Structure Depiction

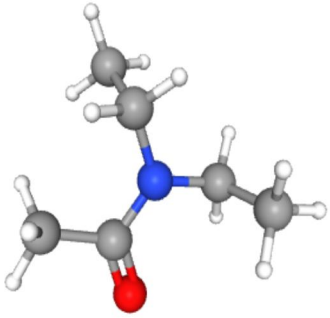


PubChem

1.2 3D Conformer

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

N,*N*-diethylacetamide

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C6H13NO/c1-4-7(5-2)6(3)8/h4-5H2,1-3H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.3 InChI Key

AJFDBNQQDYLMJN-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

CCN(CC)C(=O)C

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C6H13NO

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

685-91-6

CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Hazardous Substances Data Bank (HSDB)

2.3.2 European Community (EC) Number

211-685-2

European Chemicals Agency (ECHA)

2.3.3 NSC Number

101

DTP/NCI

2.3.4 UNII

6YO81D7ST6

FDA/SPL Indexing Data

2.3.5 DSSTox Substance ID

DTXSID9020459

EPA DSSTox

2.4 Synonyms

2.4.1 MeSH Entry Terms

N,N-diethylacetamide

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

N,N-DIETHYLACETAMIDE	NSC 101	SCHEMBL18738	AKOS003862095	119352-EP2289965A1
685-91-6	Acetic acid, amide, N,N-diethyl	N,N-Diethylacetamide, 97%	CZJT-685-91-6	119352-EP2298828A1
Acetamide, N,N-diethyl-	EINECS 211-685-2	4-04-00-00349 (Beilstein Handbook Reference)	DS-3397	Q27265731
N-Acetyldiethylamine	BRN 1209428	CH3CON(C2H5)2	NE10631	
UNII-6YO81D7ST6	AI3-02182	NSC101	NCGC00248816-01	
N,N-diethyl-acetamide	n-diethylacetamide	CHEMBL3184758	NCGC00258287-01	
MFCD00009047	N,N-diethylacetoamide	DTXSID9020459	AK105973	
6YO81D7ST6	N,N-diethylethanamide	WLN: 2N2&V1	CAS-685-91-6	
Acetamide,N,N-Diethyl-	N,N-di ethylacetamide	NSC-101	P948	
N,N-Diaethylacetamid	ACMC-20ah6c	ZINC388233	SY037752	
N,N-Diaethylacetamid [German]	DSSTox_CID_459	ADAL1185351	D0461	
N,N-diethyl acetamide	DSSTox_RID_75604	Tox21_200733	FT-0629458	
HSDB 5513	DSSTox_GSID_20459	ANW-73186	25725-EP2315303A1	

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	115.17	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	0.3	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	115.099714038	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	115.099714038	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	20.3 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	8	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	76.6	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	0	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

3.2 Experimental Properties

3.2.1 Color/Form

Colorless liquid

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 372

Hazardous Substances Data Bank (HSDB)

3.2.2 Odor

Faint odor

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 372

Hazardous Substances Data Bank (HSDB)

3.2.3 Boiling Point

185.5 °C

EPA DSSTox; Hazardous Substances Data Bank (HSDB)

3.2.4 Melting Point

LESS THAN 20 °C

Patty, F. (ed.). Industrial Hygiene and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience Publishers, 1963., p. 1830

Hazardous Substances Data Bank (HSDB)

3.2.5 Flash Point

170 °F

Hawley, G.G. The Condensed Chemical Dictionary. 9th ed. New York: Van Nostrand Reinhold Co., 1977., p. 285

Hazardous Substances Data Bank (HSDB)

3.2.6 Solubility

Sol in water, alcohol; sol in all proportions in ether, acetone, benzene

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-4

▸ Hazardous Substances Data Bank (HSDB)

3.2.7 Density

0.9130 @ 17 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-4

▸ Hazardous Substances Data Bank (HSDB)

3.2.8 Vapor Pressure

2 MM HG @ 35 °C

Patty, F. (ed.). Industrial Hygiene and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience Publishers, 1963., p. 1830

▸ Hazardous Substances Data Bank (HSDB)

3.2.9 LogP

0.34 (LogP)

HANSCH,C ET AL. (1995)

▸ EPA DSSTox

log Kow = 0.34

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 24

▸ Hazardous Substances Data Bank (HSDB)

3.2.10 Decomposition

When heated to decomposition it emits toxic fumes of /nitrogen oxides/.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

▸ Hazardous Substances Data Bank (HSDB)

3.2.11 Refractive Index

Index of refraction: 1.4374 @ 17.4 °C/4 °C

Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-4

▸ Hazardous Substances Data Bank (HSDB)

3.2.12 Kovats Retention Index

Standard non-polar	966
Semi-standard non-polar	985
Standard polar	1595

▸ NIST Mass Spectrometry Data Center

3.3 SpringerMaterials Properties

Boiling point
Chemical shift
Density
Diamagnetic susceptibility
Dielectric constant
Excess enthalpy
Heat of solution
Heat of sublimation
Optical coefficient
Refractive index
Vapor pressure
Viscosity

Hydrogen bonding potential
Lineshape
Magnetic susceptibility
Mixing enthalpy

SpringerMaterials

4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra	NMR: 6701 (Sadtler Research Laboratories Spectral Collection)

▶ Hazardous Substances Data Bank (HSDB)

1D NMR Spectra	NMRShiftDB Link

▶ NMRShiftDB

4.1.1 1H NMR Spectra

Instrument Name	Varian A-60
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 2009-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▶ SpectraBase

Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	137529
Copyright	Copyright © 2021 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▶ SpectraBase

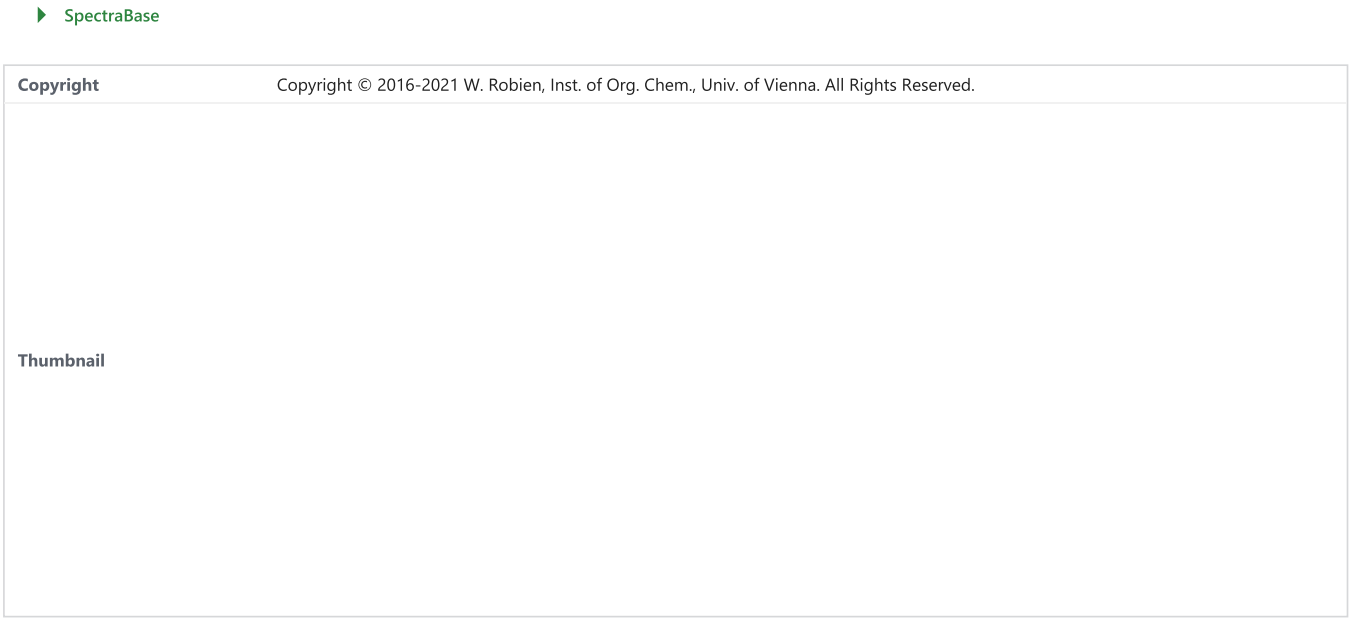
4.1.2 13C NMR Spectra

Showing 2 of 21 View More

Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin

Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



SpectraBase

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Thumbnail

SpectraBase

4.1.3 15N NMR Spectra

Instrument Name	Bruker WH-90
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Thumbnail

SpectraBase

4.1.4 17O NMR Spectra

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Thumbnail

SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

Showing 2 of 15 View More

NIST Number	233706
Library	Main library
Total Peaks	41
m/z Top Peak	58
m/z 2nd Highest	115
m/z 3rd Highest	44

Thumbnail

NIST Mass Spectrometry Data Center

NIST Number	149222
Library	Replicate library
Total Peaks	47
m/z Top Peak	58
m/z 2nd Highest	44
m/z 3rd Highest	43
Thumbnail	

NIST Mass Spectrometry Data Center

4.2.2 Other MS

Other MS	MS: NIST (NIST/EPA/MCDC Mass Spectral Database 1990 version) 1861; NBS (National Bureau of Standards) 1594

Hazardous Substances Data Bank (HSDB)

4.3 UV Spectra

MAX ABSORPTION (WATER): APPROX 200 NM (LOG E= 3.96)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-84

Hazardous Substances Data Bank (HSDB)

4.4 IR Spectra

IR Spectra	IR: 1874 (Sadtler Research Laboratories Prism Collection)

Hazardous Substances Data Bank (HSDB)

4.4.1 FTIR Spectra

Technique	Neat
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Aldrich
Catalog Number	137529
Copyright	
Thumbnail	

SpectraBase

4.4.2 ATR-IR Spectra

Source of Sample	Aldrich
Catalog Number	137529
Copyright	

Thumbnail

SpectraBase

4.4.3 Near IR Spectra

Instrument Name	BRUKER IFS 88
Technique	NIR Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=3931,REO=2,CNM=HEI,ZFF=2
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
Copyright	Copyright © 1989, 1990-2021 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

SpectraBase

Instrument Name	BRUKER IFS 88
Technique	NIR Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=3931,REO=2,CNM=HEI,ZFF=2
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
Copyright	Copyright © 1989, 1990-2021 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

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4.4.4 Vapor Phase IR Spectra

Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	137529
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4.5 Raman Spectra

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Thumbnail	

SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Related Compounds

Same Parent, Exact	18 Records
Mixtures, Components, and Neutralized Forms	80 Records
Similar Compounds	33 Records
Similar Conformers	3,046 Records

PubChem

5.3 Substances

5.3.1 Related Substances

All	218 Records
Same	113 Records
Mixture	105 Records

PubChem

5.3.2 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed	1 Record

PubChem

6 Chemical Vendors

- PubChem

7 Pharmacology and Biochemistry

7.1 Metabolism/Metabolites

IN MICE, THE DISCREPANCY BETWEEN IN VITRO & IN VIVO LIVER ENZYME INHIBITION ACTIVITY MAY BE DUE TO OXIDATIVE N-DEALKYLATION OF N,N-DIETHYLACETAMIDE OCCURRING IN VIVO, FACILITATING THE INHIBITION.

PMID:7308906

BEHYL FE, LINDNER E; FOOD COSMET TOXICOL 19 (5): 627 (1981)

Hazardous Substances Data Bank (HSDB)

8 Use and Manufacturing

8.1 General Manufacturing Information

EPA TSCA Commercial Activity Status

Acetamide, N,N-diethyl-: ACTIVE

https://www.epa.gov/tsca-inventory

▸ EPA Chemicals under the TSCA

DIETHYLACETAMIDE- AN EXAMPLE OF DRUG ABUSE.

ADERJAN R; DIETHYLACETAMIDE- AN IMPRESSIVE EXAMPLE OF DRUG ABUSE; MED WELT 30(13) 485 (1979)

▸ Hazardous Substances Data Bank (HSDB)

SOLVENTS WERE TESTED IN MICE FOR THEIR TOXICITY, CENTRAL NERVOUS SYSTEM PROFILE, AND ACTIVITY IN THE INCLINED SCREEN AND BALANCE ROD TESTS AFTER INTRAPERITONEAL ADMINISTRATION, PLUS THEIR INFLUENCE ON THE HEXABARBITONE SLEEPING TIME AND MUSCLE RELAXANT PROPERTIES ON THE ROTA-ROD AFTER ORAL ADMINISTRATION. N,N-DIETHYLACETAMIDE WAS RECOMMENDED NOT TO EXCEED A CONCENTRATION OF 0.3 IN DRUG SOLUTIONS AS SOLVENT FOR SCREENING PURPOSES.

BUDDEN R ET AL; EXPERIMENTS ON THE TOXIC, SEDATIVE AND MUSCLE RELAXANT POTENCY OF VARIOUS DRUG SOLVENTS IN MICE; PHARMACOL THER 5(1-3) 467 (1979)

▸ Hazardous Substances Data Bank (HSDB)

9 Safety and Hazards

9.1 Hazards Identification

9.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	Warning
GHS Hazard Statements	H302 (100%): Harmful if swallowed [**Warning** Acute toxicity, oral] H312 (88.64%): Harmful in contact with skin [**Warning** Acute toxicity, dermal] H315 (100%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H332 (88.64%): Harmful if inhaled [**Warning** Acute toxicity, inhalation] H335 (88.64%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P261, P264, P270, P271, P280, P301+P312, P302+P352, P304+P312, P304+P340, P305+P351+P338, P312, P321, P322, P330, P332+P313, P337+P313, P362, P363, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 45 companies from 5 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 1 of 45 companies. For more detailed information, please visit **ECHA C&L website.*** *Of the 4 notification(s) provided by 44 of 45 companies with hazard statement code(s).* *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.*

▸ European Chemicals Agency (ECHA)

9.1.2 Hazard Classes and Categories

Acute Tox. 4 (100%)

Acute Tox. 4 (88.64%)

Skin Irrit. 2 (100%)

Eye Irrit. 2A (100%)

Acute Tox. 4 (88.64%)

STOT SE 3 (88.64%)

▸ European Chemicals Agency (ECHA)

9.1.3 Fire Potential

Flammable when exposed to heat or flame.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

▸ Hazardous Substances Data Bank (HSDB)

9.2 Fire Fighting

9.2.1 Fire Fighting Procedures

To fight fire, use foam, mist, /carbon dioxide/, dry chemical.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

▸ Hazardous Substances Data Bank (HSDB)

9.3 Accidental Release Measures

9.3.1 Disposal Methods

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

Hazardous Substances Data Bank (HSDB)

9.4 Regulatory Information

9.4.1 TSCA Requirements

Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. N,N-Diethylacetamide is included on this list.

40 CFR 716.120 (7/1/2000)

Hazardous Substances Data Bank (HSDB)

9.5 Other Safety Information

9.5.1 Toxic Combustion Products

When heated to decomposition it emits toxic fumes of /nitrogen oxides/.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

Hazardous Substances Data Bank (HSDB)

10 Toxicity

10.1 Toxicological Information

10.1.1 Acute Effects

8 items View More

Organism	Test Type	Route	Dose	Effect	Reference
rat	LD50	intraperitoneal	1840 mg/kg		Arzneimittel-Forschung. Drug Research., 20(1242), 1970 [PMID:5536801]
rat	LDLo	intravenous	1 gm/kg	BEHAVIORAL: ALTERED SLEEP TIME (INCLUDING CHANGE IN RIGHTING REFLEX)	Arzneimittel-Forschung. Drug Research., 28(1571), 1978 [PMID:582558]
rat	LD50	unreported	1500 mg/kg		Arzneimittel-Forschung. Drug Research., 19(1073), 1969 [PMID:4310199]
mouse	LD50	intraperitoneal	1600 mg/kg	SENSE ORGANS AND SPECIAL SENSES: MYDRIASIS (PUPILLARY DILATION): EYE	Pharmacology and Therapeutics., 5(467), 1979
dog	LDLo	intravenous	1 gm/kg	BEHAVIORAL: ALTERED SLEEP TIME (INCLUDING CHANGE IN RIGHTING REFLEX)	Arzneimittel-Forschung. Drug Research., 28(1571), 1978 [PMID:582558]

1 2 Next

ChemIDplus

10.1.2 Interactions

CMPDS INCLUDING N,N-DIETHYLACETAMIDE SHOWED NONSPECIFIC SPASMOLYTIC PROPERTIES AGAINST HISTAMINE-, CARBACHOL-, & BARIUM CHLORIDE-INDUCED SPASMS IN ISOLATED GUINEA PIG ILEUM.

BUDDEN R ET AL; ARZNEIM-FORSCH 28 (9): 1571 (1978)

Hazardous Substances Data Bank (HSDB)

10.1.3 Antidote and Emergency Treatment

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist respirations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Activated charcoal is not effective ... . Do not attempt to neutralize because of exothermic reaction. Cover skin burns with dry, sterile dressings after decontamination ... . /Organic acids and related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 152-3

Hazardous Substances Data Bank (HSDB)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in respiratory arrest. Early intubation, at the first sign of upper airway obstruction, may be necessary. Positive pressure ventilation techniques with a bag valve mask device may be beneficial. Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start an IV with D5W /SRP: "To keep open", minimal flow rate/. Use lactated Ringer's if signs of hypovolemia are present. Watch for signs of fluid overload. Consider drug therapy for pulmonary edema ... . For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Organic acids and related compounds/

Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 153

Hazardous Substances Data Bank (HSDB)

10.1.4 Human Toxicity Excerpts

DIMETHYL ACETAMIDE HAS A RELATIVELY MODERATE HEPATOTOXIC ACTION IN OCCUPATIONALLY EXPOSED WORKERS. DUE TO SCANT KNOWLEDGE OF DIMETHYL ACETAMIDE TOXICITY, DATA RELATIVE TO SOME CMPDS WHICH PRESENT STRUCTURES & ACTION ANALOGUES TO DIMETHYL ACETAMIDE & WHOSE TOXICITY IS BETTER KNOWN ARE REPORTED AS AN APPENDIX.

PMID:5095328
CORSI GC; MED LAV 62 (1): 28 (1971)

Hazardous Substances Data Bank (HSDB)

10.1.5 Non-Human Toxicity Excerpts

THE CARCINOGENIC ACTIVITY OF DIETHYLACETAMIDE WAS STUDIED BECAUSE OF ITS ABILITY TO DENATURE PROTEINS & STRUCTURAL RESEMBLANCE TO NITROSAMINE DERIVATIVES. INGESTED, IT PRODUCED A TRANSITIONAL CELL CARCINOMA OF RAT KIDNEY & SEVERE RENAL DAMAGE. EVIDENCE DOES NOT SUPPORT THE VIEW THAT CYCLIC NITROSAMINES EXERT THEIR CARCINOGENIC ACTION VIA METAB TO DIAZOALKANES.

PMID:4285466

ARGUS MF; J NATL CANCER INST 35 (6): 949 (1965)

Hazardous Substances Data Bank (HSDB)

N,N-DIETHYLACETAMIDE 600 MG/KG GIVEN TO PREGNANT RATS ON THE 13TH OR 14TH DAYS OF GESTATION PRODUCED DIAPLACENTAL TERATOGENIC EFFECTS. THIS WAS 40% OF THE LD50 DOSE.

VON KREYBIG T ET AL; ARZNEIM-FORSCH 19 (7): 1073 (1969)

Hazardous Substances Data Bank (HSDB)

CMPDS INCLUDING N,N-DIETHYLACETAMIDE SHOWED NONSPECIFIC SPASMOLYTIC PROPERTIES AGAINST HISTAMINE-, CARBACHOL-, & BARIUM CHLORIDE-INDUCED SPASMS IN ISOLATED GUINEA PIG ILEUM, & AT LOW IV DOSES AFFECTED THE HEART RATE & BLOOD PRESSURE IN RATS, CATS, & DOGS.

BUDDEN R ET AL; ARZNEIM-FORSCH 28 (9): 1571 (1978)

Hazardous Substances Data Bank (HSDB)

IN MOUSE LIVER HOMOGENATES, N,N-DIETHYLACETAMIDE HAD NO EFFECT ON A SERIES OF LIVER MIXED-FUNCTION OXIDASE & CYTOCHROME C REDUCTASE ACTIVITIES, BUT IN VIVO (150 MG/KG, IP) IT INHIBITED THESE ACTIVITIES WITHIN 45 MIN & INCREASED HEXOBARBITAL SLEEPING TIME.

PMID:7308906

BEHYL FE, LINDNER E; FOOD COSMET TOXICOL 19 (5): 627 (1981)

Hazardous Substances Data Bank (HSDB)

INJECTIONS OF N,N-DIETHYLACETAMIDE INDUCED SOME JUMPS OF CONVULSIONS IN MICE. IT INDUCED TESTICULAR ATROPHY IN RATS. RATS GIVEN 1/20 LD50 DOSES DAILY FOR 6 WK DID NOT EXHIBIT TOXIC EFFECTS BUT DID EXHIBIT DECREASED PONDERAL GROWTH.

CAUJOLLE F ET AL; ARZNEIM-FORSCH 20 (9): 1242 (1970)

Hazardous Substances Data Bank (HSDB)

10.1.6 Non-Human Toxicity Values

LD50 Rat oral 1500 mg/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

Hazardous Substances Data Bank (HSDB)

LD50 Rat iv 1 g/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

Hazardous Substances Data Bank (HSDB)

LD50 Mouse ip 1690 mg/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

Hazardous Substances Data Bank (HSDB)

LD50 Dog iv 1 g/kg

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1146

Hazardous Substances Data Bank (HSDB)

10.2 Ecological Information

10.2.1 Soil Adsorption/Mobility

Soil Adsorption Coefficient

69.18 L/kg

EPA DSSTox

11 Literature

11.1 NLM Curated PubMed Citations

PubChem

11.2 Springer Nature References

Springer Nature

11.3 Thieme References

Thieme Chemistry

11.4 Wiley References

- Wiley

11.5 Depositor Provided PubMed Citations

- PubChem

11.6 Chemical Co-Occurrences in Literature

- PubChem

11.7 Chemical-Gene Co-Occurrences in Literature

PubChem

11.8 Chemical-Disease Co-Occurrences in Literature

PubChem

12 Patents

12.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

12.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

13 Biological Test Results

13.1 BioAssay Results

PubChem

14 Classification

14.1 Ontologies

14.1.1 MeSH Tree

- Medical Subject Headings (MeSH)

14.1.2 ChemIDplus

- ChemIDplus

14.1.3 UN GHS Classification

- UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

14.1.4 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

14.1.5 EPA DSSTox Classification

- EPA DSSTox

15 Information Sources

FILTER BY SOURCE: ALL SOURCES

1. ## CAS Common Chemistry

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   N,N-Diethylacetamide
   https://commonchemistry.cas.org/detail?cas_rn=685-91-6

2. ## ChemIDplus

   LICENSE
   https://www.nlm.nih.gov/copyright.html

   N,N-Diethylacetamide
   https://chem.nlm.nih.gov/chemidplus/sid/0000685916

   ChemIDplus Chemical Information Classification
   https://chem.nlm.nih.gov/chemidplus/

3. ## DTP/NCI

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   https://www.cancer.gov/policies/copyright-reuse

   N,N-DIETHYLACETAMIDE
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=101

4. ## EPA Chemicals under the TSCA

   LICENSE
   https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

   Acetamide, N,N-diethyl-
   https://www.epa.gov/chemicals-under-tsca

5. ## EPA DSSTox

   LICENSE
   https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

   Diethylacetamide
   https://comptox.epa.gov/dashboard/DTXSID9020459

   CompTox Chemicals Dashboard Chemical Lists
   https://comptox.epa.gov/dashboard/chemical_lists/

6. ## European Chemicals Agency (ECHA)

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

   N,N-diethylacetamide
   https://echa.europa.eu/substance-information/-/substanceinfo/100.010.624

   N,N-diethylacetamide
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/33490

7. ## Hazardous Substances Data Bank (HSDB)

   N,N-DIETHYLACETAMIDE
   https://pubchem.ncbi.nlm.nih.gov/source/hsdb/5513

8. ## FDA/SPL Indexing Data

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   https://www.fda.gov/about-fda/about-website/website-policies#linking

   6YO81D7ST6
   https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

9. ## NMRShiftDB

   https://pubchem.ncbi.nlm.nih.gov/substance/589695

10. ## NIST Mass Spectrometry Data Center

    LICENSE
    https://www.nist.gov/srd/public-law

    Acetamide, N,N-diethyl-

http://www.nist.gov/srd/nist1a.cfm

11. ## SpectraBase

N,N-DIETHYLACETAMIDE
https://spectrabase.com/spectrum/EV50tV6dzj5

ACETAMIDE, N,N-DIETHYL-
https://spectrabase.com/spectrum/AFjso4cTESb

Diethylamine AC
https://spectrabase.com/spectrum/5hJVT86IwpE

Diethylamine AC
https://spectrabase.com/spectrum/DOyhSbdvDZg

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/Aod1d250nnk

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/3nyEkeRSCem

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/3J3RAWb7rmK

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/IF2we0ARvyi

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/KmvDNTqBmDo

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/E9l0YeJiV6

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/AmLDZIru1j6

N,N-DIETHYLACETAMIDE
https://spectrabase.com/spectrum/75fPM6DPOUA

DIETHYLACETAMID
https://spectrabase.com/spectrum/2T831iJD18l

AJFDBNQQDYLMJN-UHFFFAOYSA-N
https://spectrabase.com/spectrum/H4nbLJKQcXR
https://spectrabase.com/spectrum/DmVyQ8A2oTw

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/DD2dNJ0MMlt

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/DnlK5djBpmZ

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/2r7kfQfu1pc

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/1gvoWiR7kMW

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/5CSxBlf9y6L

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/eDx9V5745f

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/BKtPVnlo4eK

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/FC5uOets25c

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/Lr6R7AsrNfV

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/GcC3wZ4jGdz

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/5fYUWM1RSh2

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/9s35UcMCCqS

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/66nIHCDAqKv

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/AplYBs6Wvbj

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/Lbl24WatdLQ

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/HHHRJawC2wG

N,N-Diethylacetamide
https://spectrabase.com/spectrum/3YmWkoGNQN9

N,N-diethylacetamide
https://spectrabase.com/spectrum/3pnEYmdLqX2

N,N-Diethylacetamide
https://spectrabase.com/spectrum/FlL4IxRcXgu

N,N-DIETHYL-ACETAMIDE
https://spectrabase.com/spectrum/LS1PgzCAnZA

ACETAMIDE, N,N-DIETHYL-,
https://spectrabase.com/spectrum/A0kavyzhF0Y

N,N-Diethylacetamide
https://spectrabase.com/spectrum/5W6fELgRV0S

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/J1lBCSFf8St

Acetamide, N,N-diethyl-
https://spectrabase.com/spectrum/DqvA3q9k5rg

N,N-Diethylacetamide
https://spectrabase.com/spectrum/ELkzAoXwYB0

N,N-Diethylacetamide
https://spectrabase.com/spectrum/3K3wn5fG2bR

N,N-Diethylacetamide
https://spectrabase.com/spectrum/2rSW7AqiwaV

Methyl-N,N-diethyl-formamide
https://spectrabase.com/spectrum/JxgF9YDJQOx

12. ## Springer Nature
https://pubchem.ncbi.nlm.nih.gov/substance/341152359

13. ## SpringerMaterials
N,N-diethylacetamide
https://materials.springer.com/substanceprofile/docs/smsid_udyyzvryfpwglosg

14. ## Thieme Chemistry

15. ## Wiley
https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=41353

16. ## PubChem
https://pubchem.ncbi.nlm.nih.gov

17. ## Medical Subject Headings (MeSH)

N,N-diethylacetamide
https://www.ncbi.nlm.nih.gov/mesh/67032711

MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html

18. ## UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)
GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

19. ## NORMAN Suspect List Exchange

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

20. ## PATENTSCOPE (WIPO)
SID 403030007
https://pubchem.ncbi.nlm.nih.gov/substance/403030007