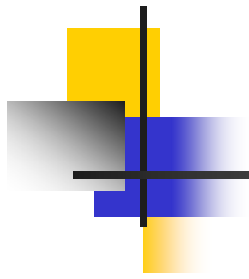


TOXNET

Toxicology and Environmental Health Information

from the National Library of Medicine (NLM)

and Other Sites



Presented by

NLM's Toxicology and Environmental Health Information Program

part of the Division of Specialized Information Services

Contact:

Toxicology and Environmental Health Information Program

Division of Specialized Information Services

National Library of Medicine

Suite 510, MSC 5467

6707 Democracy Blvd.

Bethesda, MD 20892-5467

301-496-1131

301-480-3537 (FAX)

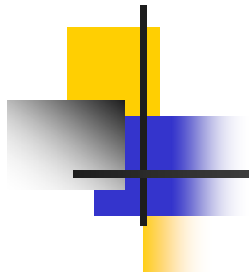
Web site: <http://sis.nlm.nih.gov/>

Contact: tehip@teh.nlm.nih.gov

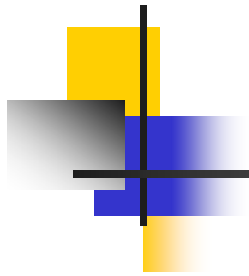


Class Schedule

Part I	Introduction	9:00 - 9:15
Part II	TOXNET Overview, HSDB & Related Files	9:15 - 10:15
	<i>Break</i>	10:15 - 10:30
	Exercises (II)	10:30 - 11:00
Part III	TOXLINE and Other Bibliographic Files	11:00 - 11:30
	Exercises (III)	11:30 - 12:00
	<i>Lunch</i>	12:00 - 1:00
Part IV	TRI, Specialty Files, New Initiatives	1:00 - 1:45
	Exercises (IV)	1:45 - 2:15
Part V	Non-NLM Resources	2:15 - 2:45
	<i>Break</i>	2:45 - 3:00
Part VI	ChemIDplus	3:00 - 3:30
	Exercises (V, VI)	3:30 - 4:00



Class List



Part I

Introduction



Toxicology and Environmental Health Information Program (TEHIP)

Background

- Poisons recognized throughout time.
- Socrates - hemlock. Cleopatra - asp.
- Lucretia Borgia
- Harvey W. Wiley's Poison Squad – 1903
- The Jungle (1906) Upton Sinclair – lack of hygiene in the meat-packing industry
- Food and Drugs Act (1906) – prohibited adulterated or misbranded items
- Federal Food, Drug and Cosmetic Act (1938) – enhanced safety requirements for drugs
- Drug Amendments (1962) – effectiveness required for drugs
- Silent Spring (1962) Rachel Carson – sparked public awareness about hazards of synthetic chemicals
- President's Science Advisory Committee (1966) – “Report on the Handling of Toxicological Information”
- TEHIP Created (1967)
- Situated within NLM's Division of Specialized Information Services



TEHIP Mission

- Provide selected core toxicology and environmental health information resources and services
- Facilitate access to national and international toxicology and environmental health information resources
- Strengthen the information infrastructure of toxicology and environmental health

So...TEHIP

- Builds and/or makes available free online Web-based databases
- Creates other Web-based resources
- Collaborates with government agencies and others
- Is active in public training and outreach



TEHIP Databases

- TOXNET System of Databases (including ChemID*plus* and Specialty Databases)
- DIRLINE (directory of organizations)

Additional TEHIP Resources

- Special Topic Guides – arsenic, biological & chemical warfare agents, etc.
- Publications (including Glossary of Terms Used in Toxicology)
- ALTBIB - Alternatives Bibliography
- Toxicology Tutor

Other Relevant NLM Information

- PubMed/MEDLINE
- MedlinePlus (consumer health, includes drug information)
- Clinical Trials
- NLM Gateway – Multi-File Searching – Planned to go across all NLM Files



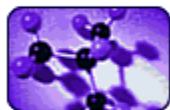
About

The Specialized Information Services (SIS) Division of the National Library of Medicine (NLM) is responsible for information resources and services in toxicology, environmental health, chemistry, HIV/AIDS, and specialized topics in minority health.



Toxicology & Environmental Health

Databases and other resources related to toxicology and environmental health. Features [TOXNET](#).



Chemical Information

Databases and other resources designed to help you search for information by chemical name or structure. Features [ChemIDplus](#).



HIV / AIDS

Links to journal literature, clinical trials and treatment information, meeting abstracts, and other scientific and consumer-related resources.



Directory of Health Organizations

Features [DIRLINE](#) and [Health Hotlines](#).

More to Explore

[News](#)
[Outreach Activities](#)
[Staff Directory](#)
[Site Map and Search](#)
[Fact Sheets](#)

[Review of PDA Applications in Toxicology and Environmental Health](#) **NEW**

[International Toxicity Estimates for Risk \(ITER®\)](#) **NEW**

[NLM Environmental Health and Toxicology Listserv](#)

[Household Products Database](#)

[Asian American Health Web Site](#)

[AIDSinfo](#)



Toxicology and Environmental Health

TOXNET

Databases in toxicology and environmental health.

TOXLINE	HSDB	ChemIDplus
DART	TRI	IRIS
GENE-TOX	CCRIS	ITER NEW

Internet Resources

Evaluated links to Internet resources on current issues such as [chemical warfare agents](#) and [Environmental Justice](#).

Haz-Map

Database on hazardous chemicals and occupational diseases.

ALTBIB

References about alternatives to the use of live animals in biomedical research and testing.

Toxicology Tutor

Three self-guided tutorials on toxicology.

News and Events

Links to news items on the web site, [outreach activities](#) and a [calendar of events](#).

Review of PDA Applications in Toxicology and Environmental Health **NEW**

A descriptive review of selected applications for PDAs covering toxicology and environmental health.

NLM Listserv on Environmental Health and Toxicology Information

An [email list](#) announcing updates in SIS's resources, services, and outreach in toxicology and environmental health.

Consumer Health

[Tox Town](#)

An interactive guide to commonly encountered toxic substances.

[Household Products Database](#)

Health & safety information on consumer household products.

[MedlinePlus](#)

[Poisoning, Toxicology and Environmental Health](#)

[DIRLINE](#)

Over 10,000 health organizations.

[Health Hotlines](#)

Toll-free numbers to 300 organizations.

MEDLINE/PubMed

References from more than 4,600 biomedical journals, including the [Toxicology Subset](#).

Other Resources

[Chemical Information](#)

[Selected Toxicology Links](#)

- [10th Report on Carcinogens](#) (National Toxicology Program)
- [Second National Report on Human Exposure to Environmental Chemicals](#) (Centers for Disease Control and Prevention)

[Reference Material](#)

Bibliographies, glossary, reports.

[Database descriptions](#)

[TOXNET Manual](#)

[Locatorplus](#)

The NLM catalog of books, journals, and audiovisuals.

[NLM Gateway](#)

Search multiple databases at NLM.



Directory of Health Organizations Online

[▶ Directory of Health Organizations ▶](#)
DIRLINE

[Search DIRLINE](#)

[Other NLM Resources](#)

Search:

all of the words any of the words exact phrase

Fields: (if none checked, all fields will be searched.)

Organization name or acronym

MeSH Headings/Keywords

Select records containing:

Only organizations with toll-free numbers

Only organizations with services for the hearing impaired

[Health Hotlines](#)

[MEDLINEplus](#)

[PubMed](#)

[NLM Gateway](#)

[Locatorplus](#)

[Support Page](#)

[Fact Sheet](#)

[Disclaimer](#)

[Suggestion Form](#)



DIRLINE Search Results

[Directory of Health Organizations](#)

[DIRLINE](#)

Save
Checked Items

Sort

Details

History

Download

Modify Search

New Search

Download

Modify Search

New Search

Download

Modify Search

New Search

Browse Index

SIS
Home

MEDLINEplus
Home

drinking water

Search

Clear

Items 1 through 20 of 46

Pages: [1](#) [2](#) [3](#)

Organization Names are sorted in *relevancy ranked* order.

Select Record	Organization Name
1 <input type="checkbox"/>	Drinking Water Program - Massachusetts Department of Environmental Protection
2 <input type="checkbox"/>	National Drinking Water Clearinghouse - National Environmental Service Center - West Virginia University (NDWC)
3 <input type="checkbox"/>	Office of Ground Water and Drinking Water - U.S. Environmental Protection Agency (OGWDW)
4 <input type="checkbox"/>	Division of Drinking Water - Virginia Department of Health (DDW)
5 <input type="checkbox"/>	Drinking Water Program - Division of Drinking Water and Environmental Management - California Department of Health Services - California State Government (DWP)
6 <input type="checkbox"/>	Water Supply and Water Resources Division - National Risk Management Research Laboratory - U.S. Environmental Protection Agency
7 <input type="checkbox"/>	Office of Water Quality - Indiana Department of Environmental Management - Indiana State Government (OWQ)
8 <input type="checkbox"/>	American Water Works Association (AWWA)
9 <input type="checkbox"/>	Office of Drinking Water Quality - Rhode Island Department of Health
10 <input type="checkbox"/>	Office of Water - U.S. Environmental Protection Agency (OW)
11 <input type="checkbox"/>	Water Environment Federation (WEF)
12 <input type="checkbox"/>	Clean Water Action (CWA)
13 <input type="checkbox"/>	WATERNET - American Water Works Association



Poisoning, Toxicology, Environmental Health Topics

- [Air Pollution](#)
- [Anthrax](#)
- [Arsenic](#)
- [Asbestos](#)
- Asbestosis see [Asbestos](#)

- [Biodefense and Bioterrorism](#)
- Biological Weapons see [Biodefense and Bioterrorism](#)
- Bioterrorism see [Biodefense and Bioterrorism](#)
- Campylobacter see [Food Contamination and Poisoning](#)
- [Carbon Monoxide Poisoning](#)

- Cell Phones see [Electromagnetic Fields](#)
- [Chemical Weapons](#)
- Cleaning Products see [Household Poisons](#)
- [Drinking Water](#)
- EMF see [Electromagnetic Fields](#)

- [Electromagnetic Fields](#)
- [Environmental Health](#)
- Environmental Tobacco Smoke see [Secondhand Smoke](#)
- [Food Contamination and Poisoning](#)
- Food Poisoning see [Food Contamination and Poisoning](#)

- [Food Safety](#)
- Fungicides see [Pesticides](#)
- Germ Warfare see [Biodefense and Bioterrorism](#)
- Hazardous Waste see [Environmental Health](#)
- Herbicides see [Pesticides](#)

[Browse](#) : [By Condition](#) : [By Disease Heading](#) : [Injuries, Poisonings, and Occupational Diseases](#) : **Disorders of Environmental Origin**

Include trials that are no longer recruiting patients.

Search-Within-Results

Query Details

Map of locations

123 studies were found. Here are studies 1 to 50. [Next 50](#)

- Recruiting** [Reducing Pesticide Exposure in Minority Families](#)
Condition: Disorders of Environmental Origin
- Recruiting** [Serotonin in Alcoholism](#)
Conditions: Alcoholism; Healthy
- Recruiting** [Pesticide Exposure Pathways for Farmworker Children](#)
Condition: Poisoning
- Recruiting** [Brain Function in Children Previously Treated on Clinical Trials POG-9605 and POG-9201](#)
Conditions: neurotoxicity, long-term effects secondary to cancer therapy in children
- Recruiting** [Prevention of Violent Behavior Among Children](#)
Conditions: Aggression; Violence; Wounds and Injuries
- Recruiting** [Adjuvant Nutrition for Critally Ill Trauma Patients](#)
Condition: Trauma
- Recruiting** [Phase II Randomized Study of Cultured Skin Substitutes versus Split Thickness Skin Grafts in Patients with Severe Burn Injuries](#)
Condition: Burns
- Recruiting** [Randomized Study of Testosterone and Progressive Resistance Exercise in Men With Burn Injury](#)
Condition: Burns
- Recruiting** [Environmental Contaminants and Infant Development](#)
Conditions: Mercury Poisoning; Lead Poisoning
- Recruiting** [Follow-up of Psychological and Neurocognitive Gulf War Outcome: Relation to Stress](#)
Condition: Gulf War Syndrome



Gateway

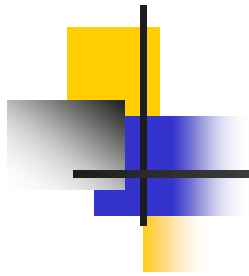
your entrance to the
knowledge resources of the
National Library of Medicine

New Search

[Overview](#)[What's New](#)[Help](#)[F A Q](#)[Other NLM Resources](#)[Ordering Info.](#)[Clinical Alerts](#)[ClinicalTrials.gov](#)[HSTAT](#)[LOCATORplus](#)[MEDLINEplus](#)[PubMed](#)[TOXNET](#)

Results Summary

Category	Items Found	Actions	
Journal Citations	5062	<input type="button" value="Display Results"/>	<input type="button" value="Details of Search"/>
Books / Serials / AVs	27	<input type="button" value="Display Results"/>	<input type="button" value="Details of Search"/>
Consumer Health	223	<input type="button" value="Display Results"/>	<input type="button" value="Details of Search"/>
Meeting Abstracts	3	<input type="button" value="Display Results"/>	<input type="button" value="Details of Search"/>
Other Collections	379	<input type="button" value="Display Results"/>	<input type="button" value="Details of Search"/>
Total	5694		



Part II

TOXNET Overview, HSDB, & Related Files



What is TOXNET?

- A free web-based system of databases on toxicology, environmental health, hazardous chemicals, toxic releases, chemical nomenclature, and specialty areas such as occupational health and consumer products
- A product of NLM's Toxicology and Environmental Health Information Program
- Toxicology Data (one record per chemical)– HSDB, IRIS, CCRIS, GENE-TOX, ITER (can also search any combination of these files with “Multi-Databases” interface)
- Toxicology Literature (bibliographic references) – TOXLINE, DART/ETIC
- Toxic Releases (of chemicals to the environment) – TRI
- Chemical Identification/Nomenclature – ChemIDplus
- Specialty Databases – HazMap, Household Products
- User Support – tehip@teh.nlm.nih.gov or click on “Contact TOXNET”

Where is TOXNET?

toxnet.nlm.nih.gov



TOXNET

▶ [Tox. & Env. Health](#) ▶ [TOXNET](#)

Welcome to TOXNET, a cluster of databases on toxicology, hazardous chemicals, and related areas.

Databases

HSDB	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i

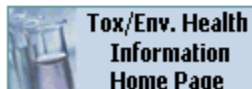
Search All Databases

Other NLM Resources

- [Tox/Env. Health Home Page](#)
- [Haz-Map](#)
- [Tox Town](#)
- [Household Products Database](#)
- [ALTBIB](#)
- [MEDLINEplus Tox/Env. Health](#)
- [MEDLINE/PubMed](#)
- [DIRLINE](#)
- [NLM Gateway](#)

Support Pages

- [Help](#)
- [Database Descriptions](#)
- [News](#)
- [2002 TOXNET Survey Results](#)



**Tox/Env. Health
Information
Home Page**



TOXNET

[Tox. & Env. Health](#) [TOXNET](#)

Welcome to TOXNET, a cluster of databases on toxicology, hazardous chemicals, and related areas.

Databases

HSDB	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i

Search All Databases

Search Results:

Database	Records found i
TOXLINE Special	3554
DART Special	71
HSDB	75
IRIS	1
ITER	1
GENETOX	1
CCRIS	1
TRI	7
CHEMIDplus	1

Other NLM Resources

- [Tox/Env. Health Home Page](#)
- [Haz-Map](#)
- [Tox Town](#)
- [Household Products Database](#)
- [ALTBIB](#)
- [MEDLINEplus Tox/Env. Health](#)
- [MEDLINE/PubMed](#)
- [DIRLINE](#)
- [NLM Gateway](#)

Support Pages

- [Help](#)
- [Database Descriptions](#)
- [News](#)
- [2002 TOXNET Survey Results](#)



Toxicology Data Files - Content

Hazardous Substances Data Bank (HSDB) – from NLM

4784 Chemical Records

Human Health Effects

Emergency Medical Treatment

Animal Toxicity Studies

Metabolism/Pharmacokinetics

Pharmacology

Environmental Fate/Exposure

Environmental Standards & Regulations

Chemical/Physical Properties

Chemical Safety & Handling

Occupational Exposure Standards

Manufacturing and Use

Laboratory Methods

Special References

Synonyms and Identifiers



More about HSDB

- Factual Data Bank/Online Handbook
- Peer-Reviewed – Scientific Review Panel
- Review Status Tags – Peer Reviewed, QC Reviewed, Unreviewed
- Fully Referenced
- Data – Excerpted from books, government documents, technical reports, selected primary literature, databases. Some data compiled expressly for HSDB.



Toxicology Data Files - Content

Chemical Carcinogenesis Research Information System (CCRIS) –
from the National Cancer Institute (NCI)
8903 Chemical Records

Carcinogenicity Studies

Tumor Inhibition Studies

Tumor Promotion Studies

Mutagenicity Studies

e.g. Carcinogenicity Studies Data Structure – species, route, tumor site/type of lesion, results, reference



Toxicology Data Files - Content

GENE-TOX

from the U.S. Environmental Protection Agency (EPA)

3214 Chemical Records

Note: GENE-TOX not updated since January 2000

Mutagenicity Studies

Data Structure – assay type, assay code, results, panel report, reference



Toxicology Data Files - Content

Integrated Risk Information System (IRIS)

from the U.S. Environmental Protection Agency (EPA)

542 Chemical Records

Noncarcinogenic Assessment – Oral (RfD) Carcinogenic Assessment - Oral

Noncarcinogenic Assessment – Inhalation (RfC) Carcinogenic Assessment -
Inhalation

- Contains EPA consensus scientific positions and quantitative values on cancer and non-cancer health effects that may result from lifetime oral or inhalation exposure to specific chemical substances in the environment
- Risk Assessment – Identification and quantification of risk. Function of toxicity and exposure
- Risk Assessment Process (National Academy of Sciences, 1983) – 1. Hazard identification, 2. Dose-Response assessment [IRIS], 3. Exposure assessment, 4. Risk Characterization



Toxicology Data Files - Content

International Toxicity Estimates for Risk Assessment (ITER) from the Toxicology Excellence for Risk Assessment (TERA) 616 Chemical Records

Tabular and Comparative Risk Data for Cancer Oral, Non-Cancer Oral, Cancer Inhalation, Non-Cancer Inhalation Effects from:

Agency for Toxic Substances and Disease Registry, U.S. (ATSDR)

Environmental Protection Agency, U.S. (EPA)

Health Canada

International Agency for Research on Cancer (IARC)

NSF International (National Sanitation Foundation)

National Institute of Public Health and the Environment, Dutch (RIVM)

Independently-derived Values

Includes synopses, links to organization source documents



TOXNET Search Screen Options

- TOXNET Home Page Search
 - Single query box search
 - No limits
 - Gives quick counts of records retrieved and allows links to each database
 - Number of records retrieved in each database may vary from numbers attained by searching databases directly

- Database specific searches – interface varies according to type of database

- Multi-Databases search – interface for any combination of data files (i.e. HSDB, CCRIS, GENE-TOX, IRIS, ITER)



Search Page - Toxicology Data Files

- One Box Search for:
 - Chemicals – enter chemical names or CAS Registry numbers. System add synonyms (default) or use exact terms entered.
 - Other Terms


- Browse Index for:
 - All Words
 - Chemical name
 - CAS Registry Number

- Limits
 - For more precise searching – searching for terms within particular data fields



Search Results Page -Toxicology Data Files

- Displays chemical names and registry numbers of retrieved records
- Relevancy Ranked Display
- Select Record(s) of Interest
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a New Search – Returns you to Search Page with blank query box
- Or Search can be modified or begun anew directly on Results Page
- Sort Results – By substance name, ascending or descending sequence
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Entire Record(s) or Custom Format
- Browse Index
- Get Help
- Return to TOXNET Home



Selected Record Page - Toxicology Data Files

Default display varies

- Chemical Search – HSDB displays human health effects, other files display full record
- Other Term(s) Search – Best Sections
- **Search Term(s) Highlighted in Red**
- Choose fields for display from Contents (expand, contract categories)
- Navigate – Next Item, Previous Item
- View Details of Search Strategy
- Modify Search – Returns you to Search Screen with query intact
- Begin a New Search – Returns you to Search Screen with blank query box
- Download – Entire Record(s) or Custom Format
- Browse Index
- Get Help
- Return to TOXNET Home
- Link to records for the same chemical in Other Files - (including TOXLINE and ChemID*plus*)



Hazardous Substances Data Bank

[▶ Tox. & Env. Health](#) [▶ TOXNET](#) [▶ HSDB](#)

Databases

Hazardous Substances Data Bank	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i
TOXNET Home	

Search HSDB

For chemicals, add synonyms and CAS numbers to search:

Yes
 No

Other NLM Resources

- [Tox/Env. Health Home Page](#)
- [Haz-Map](#)
- [Tox Town](#)
- [Household Products Database](#)
- [ALTBIB](#)
- [MEDLINEplus Tox/Env. Health](#)
- [MEDLINE/PubMed](#)
- [DIRLINE](#)
- [NLM Gateway](#)

Support Pages

- [Help](#)
- [Fact Sheet](#)
- [Sample Record](#)
- [HSDB Scientific Review Panel](#)



HSDB Search Results

▶ [Tox. & Env. Health](#) ▶ [TOXNET](#) ▶ [HSDB](#)

- Save Checked Items
- Sort
- Details
- History
- Download
- Modify Search
- Basic Search
- Download
- Modify Search
- Basic Search
- Download
- Modify Search
- Basic Search
- Browse Index
- Help
- TOXNET Home

For chemicals, add synonyms and CAS numbers to search: Yes No

Items 1 through 20 of 1943

Page 1 of 98. to page

Substance Names are sorted in *relevancy ranked* order.

Select Record	Substance Name
---------------	----------------

The following is the primary record for the chemical. All of the query terms were found.

1 [ACETONE](#)
67-64-1

The following 1942 records contain one or more of the requested chemical name(s) and all of the query terms anywhere in the record.

2 [ACETONE CYANOHYDRIN](#)
75-86-5

3 [1-CHLORO-2-PROPANONE](#)
78-95-5

4 [ISOPROPANOL](#)
67-63-0













5 [1,1,1,3,3,3-HEXAFLUORO-2-PROPANONE](#)
684-16-2

Contents

Contract all categories Expand all categories

Select

Clear

-  [FULL RECORD](#)
-  [Human Health Effects](#)
-  [Emergency Medical Treatment](#)
-  [Animal Toxicity Studies](#)
-  [Metabolism/Pharmacokinetics](#)
-  [Pharmacology](#)
-  [Environmental Fate & Exposure](#)
-  [Environmental Standards & Regulations](#)
-  [Chemical/Physical Properties](#)
-  [Chemical Safety & Handling](#)
-  [Occupational Exposure Standards](#)
-  [Manufacturing/Use Information](#)
-  [Laboratory Methods](#)
-  [Special References](#)
-  [Synonyms and Identifiers](#)
-  [Administrative Information](#)

ACETONE

CASRN: 67-64-1

For other data, click on the Table of Contents

Click to see other databases
with acetone records

Human Health Effects:**Toxicity Summary:**











Exposure to **acetone** results from both natural and anthropogenic sources. **Acetone** also occurs as a metabolic component in blood, urine and human breath. ... **Acetone** is one of three ketone bodies that occur naturally throughout the body. It can be formed endogenously in the mammalian body from fatty acid oxidation. Fasting, diabetes mellitus and strenuous exercise increase endogenous generation of **acetone**. Under normal conditions, the production of ketone bodies occurs almost entirely within the liver and to a smaller extent in the lung and kidney. ... Products are excreted in the blood and transported to all tissues and organs of the body where they can be used as a source of energy. Two of these ketone bodies, acetoacetate and beta-hydroxybutyrate, are organic acids that can cause metabolic acidosis when produced in large amounts, as in diabetes mellitus. ... Endogenous **acetone** is eliminated from the body either by excretion in urine and exhaled air or by enzymatic metabolism. ... **Acetone** is rapidly absorbed via the respiratory and gastrointestinal tracts of human and laboratory animals, as indicated by the detection of **acetone** in blood within 30 min of inhalation exposure and 20 min of oral administration. ... The nasal cavities of human and laboratory animals appear to have a limited ability to absorb and excrete **acetone** vapor, compared with the remainder of the respiratory tract. **Acetone** is uniformly distributed among non-adipose tissues and does not accumulate in adipose tissue. ... **Acetone** is rapidly cleared from the body by metabolism and excretion. ... Exhalation is the major route of elimination for **acetone** and its terminal metabolite (carbon dioxide), and the fraction of administered **acetone** that is exhaled as unchanged **acetone** is dose-related. Urinary excretion of **acetone** and its metabolites occurs but this route of elimination is minor ... Exogenously supplied **acetone**

Contents

Contract all categories Expand all categories

Select

Clear

-  [FULL RECORD](#)
-  [Human Health Effects](#)
-  [Emergency Medical Treatment](#)
-  [Animal Toxicity Studies](#)
-  [Metabolism/Pharmacokinetics](#)
-  [Pharmacology](#)
-  [Environmental Fate & Exposure](#)
-  [Environmental Standards & Regulations](#)
-  [Chemical/Physical Properties](#)
-  [Chemical Safety & Handling](#)
-  [Occupational Exposure Standards](#)
-  [Manufacturing/Use Information](#)
-  [Laboratory Methods](#)
-  [Special References](#)
-  [Synonyms and Identifiers](#)
-  [Administrative Information](#)

ACETONE

CASRN: 67-64-1


*For other data, click on the Table of Con***Human Health Effects:****Toxicity Summary:**

Exposure to **acetone** results from both natural and anthropogenic sources. **Acetone** also occurs as a metabolic component in blood, urine and human breath. ... **Acetone** is one of three ketone bodies that occur naturally throughout the body. It can be formed endogenously in the mammalian body from fatty acid oxidation. Fasting, diabetes mellitus and strenuous exercise increase endogenous generation of **acetone**. Under normal conditions, the production of ketone bodies occurs almost entirely within the liver and to a smaller extent in the lung and kidney. ... Products are excreted in the blood and transported to all tissues and organs of the body where they can be used as a source of energy. Two of these ketone bodies, acetoacetate and beta-hydroxybutyrate, are organic acids that can cause metabolic acidosis when produced in large amounts, as in diabetes mellitus. ... Endogenous **acetone** is eliminated from the body either by excretion in urine and exhaled air or by enzymatic metabolism. ... **Acetone** is rapidly absorbed via the respiratory and gastrointestinal tracts of human and laboratory animals, as indicated by the detection of **acetone** in blood within 30 min of inhalation exposure and 20 min of oral administration. ... The nasal cavities of human and laboratory animals appear to have a limited ability to absorb and excrete **acetone** vapor, compared with the remainder of the respiratory tract. **Acetone** is uniformly distributed among non-adipose tissues and does not accumulate in adipose tissue. ... **Acetone** is rapidly cleared from the body by metabolism and excretion. ... Exhalation is the major route of elimination for **acetone** and its terminal metabolite (carbon dioxide), and the fraction of administered **acetone** that is exhaled as unchanged **acetone** is dose-related. Urinary excretion of **acetone** and its metabolites occurs but this route of elimination is minor ... Exogenously supplied **acetone**





Links to Related Records in Oth...

- [IRIS Record](#)
- [CCRIS Record](#) ←
- [GENETOX Record](#)
- [TOXLINE SPECIAL Records](#)
- [TOXLINE CORE Records](#)
- [ChemIDplus Chemical Structure](#)

Contents

Contract all categories Expand all categories 

Select Clear

-  [FULL RECORD](#)
-  [Substance Identification](#)
-  [Studies Data](#)
-  [Administrative Information](#)

ACETONE

CASRN: 67-64-1

*For other data, click on the Table of Contents***Substance Identification:**

Substance Name: ACETONE

CAS Registry Number: **67-64-1****Data Type:**

Mutagenicity

Studies Data:**Mutagenicity Studies:**

Test System: AMES SALMONELLA TYPHIMURIUM
Strain Indicator: TA100
Metabolic Activation: NONE
Method: PREINCUBATION
Dose: 100-10000 UG/PLATE (TEST MATERIAL SOLVENT: DISTILLED WATER)
Results: NEGATIVE
Reference:

[ZEIGER,E, ANDERSON,B, HAWORTH,S, LAWLOR,T AND MORTELMANS,K; SALMONELLA MUTAGENICITY TESTS. V. RESULTS FROM THE TESTING OF 311 CHEMICALS; ENVIRON. MOL. MUTAGEN. 19(SUPPL.21):2-141, 1992]

Test System: AMES SALMONELLA TYPHIMURIUM
Strain Indicator: TA100
Metabolic Activation: HAMSTER, LIVER, S-9, AROCLOR 1254 (10 OR 30%)
Method: PREINCUBATION
Dose: 100-10000 UG/PLATE (TEST MATERIAL SOLVENT: DISTILLED WATER)
Results: NEGATIVE
Reference:

[ZEIGER,E, ANDERSON,B, HAWORTH,S, LAWLOR,T AND MORTELMANS,K; SALMONELLA MUTAGENICITY TESTS. V. RESULTS FROM THE TESTING OF 311 CHEMICALS; ENVIRON. MOL. MUTAGEN. 19(SUPPL.21):2-141, 1992]



“Details” of the Acetone Search

Query:

(acetone OR “dimethyl ketone” OR propanone OR “methyl ketone” OR “ketone propane”)

The chemical name **acetone** was identified.

The following terms were added from ChemIDplus:

dimethyl ketone


propanone

methyl ketone


ketone propane

CAS Registry Number: **67-64-1**

LIMITS











 **National Library of Medicine**
Specialized Information Services

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SIS 

Hazardous Substances Data Bank [Tox. & Env. Health](#) [TOXNET](#) [HSDB](#) [Limits](#)

Databases

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- [IRIS](#) 
- [ITER](#) 
- [GENE-TOX](#) 
- [CCRIS](#) 
- [Multi-Databases](#) 
- [TOXLINE](#) 
- [DART/ETIC](#) 
- [TRI](#) 
- [ChemIDplus](#) 
- [TOXNET Home](#)

Other NLM Resources

- [Tox/Env. Health Home Page](#)
- [Haz-Map](#)
- [Tox Town](#)
- [Household Products Database](#)
- [ALTBIB](#)
- [MEDLINEplus Tox/Env. Health](#)
- [MEDLINE/PubMed](#)
- [DIRLINE](#)
- [NLM Gateway](#)

Support Pages

















- [Help](#)
- [Fact Sheet](#)
- [Sample Record](#)
- [HSDB Scientific Review Panel](#)

Search HSDB

Add chemical synonyms and CAS numbers to search:
 Yes No

Search: exact words singular & plural forms word variants
Search records with: the phrase all words any words

Search in fields:
(If no box is checked, all fields will be searched.)

-  **Substance Identification**
-  **Human Health Effects**
-  **Emergency Medical Treatment**
-  **Animal Toxicity Studies**
-  **Metabolism/Pharmacokinetics**
-  **Pharmacology**
-  **Environmental Fate & Exposure**
-  **Environmental Standards & Regulations**
-  **Chemical/Physical Properties**
-  **Chemical Safety & Handling**
-  **Occupational Exposure Standards**
-  **Manufacturing/Use Information**
-  **Laboratory Methods**
-  **Special References**
-  **Synonyms and Identifiers**
-  **Administrative Information**

Search History

- To review search strategies
- To combine search statements (within databases)
- Query Box provided to enter subsequent searches directly on Search History Page
- Use # to combine search statements (e.g. #1 AND #2)

Search *HSDB* for

- Search History will be lost after one hour of inactivity.
- To combine searches use # before search number. e.g. #2 AND #6.
- Searches may not be combined across databases.

Search	Database	Query	Time	Result
# 2	hsdb	[use] [mfs] [mnmfg] [omin] [form] [imp] [cpat] [prod] [impt] "latex paint" [expt]	10:12:24	19
# 1	hsdb	[tox] [care] [htox] [htxv] [seri] [warn] [meds] [popl] [rtex] [body] [avdi] "lymphatic leukemia" [rinf]	10:12:03	5

Clear History



Boolean Searching, Field Qualification, Search Techniques

- Upper Case Boolean Operators (AND, OR, NOT)
- Fields in brackets and post-qualified (e.g. benzene [na])
- Nested parenthesis permitted
- Phrase searching with quotation marks (e.g. “coronary artery bypass”)
- Asterisk (*) for truncation (e.g. carcinogen*)

LinkOut from PubMed to HSDB

1: Chest. 2003 Nov;124(5):1716-23.

[Related Articles](#), [Links](#)

Full text article at
www.chestjournal.org

Long-term intermittent exposure to high ambient CO₂ causes respiratory disturbances during sleep in submariners.

Margel D, White DP, Pillar G.

Israeli Naval Medical Department, Haifa, Israel.

BACKGROUND: During most of the cruise, submarines are detached from their environment. Therefore, O₂ levels are relatively low (19 kPa, 144 mm Hg) and CO₂ levels are high (1 kPa, 7.6 mm Hg). There are, however, periods during ventilation of the submarine in which CO₂ levels drop and O₂ levels increase. The objective of this study was to determine whether these unique gas changes might result in sleep-disordered breathing in submariners. **METHODS AND MATERIALS:** The sleep of eight healthy soldiers was assessed three times: (1) control night, in submarine docking; (2) at the beginning of the cruise (reflecting acute exposure to gas changes); and (3) at the end of the cruise (chronic exposure to gas changes). Each night was divided to three parts because of different CO₂ levels (secondary to ventilation of the submarine). Sleep and breathing were measured using the portable Watch PAT100 device (Itamar Medical, Ltd; Caesarea, Israel) to detect breathing abnormalities during sleep. **RESULTS:** Sleep and breathing data were categorized according to four CO₂ conditions: acute moderate (inhaled CO₂ levels of 2.3 to 5 mm Hg during first 1 to 2 nights of the cruise); acute high (inhaled CO₂ levels of 5 to 9.2 mm Hg during the first 1 to 2 nights of the cruise); chronic moderate (inhaled CO₂ levels of 2.3 to 5 mm Hg during nights 9 to 10 of the cruise); and chronic high (inhaled CO₂ levels of 5 to 9.2 mm Hg during nights 9 to 10 of the cruise). Respiratory disturbance index (RDI) was significantly higher in the chronic moderate CO₂ condition than the chronic high condition (18.9/h significant), but significantly negatively correlated with it during the submariners adapt to high CO₂ levels, as evidenced by the significant increase in RDI when CO₂ levels declined during the

PMID: 14605040 [PubMed - indexed for MEDLINE]

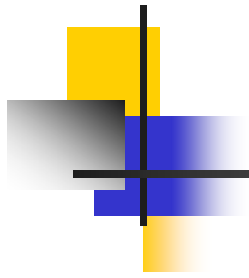
Display Show: Sort Send to

- Links to full-text and resource information are supplied by [LinkOut](#) providers.
- Links with an asterisk indicate the LinkOut provider requires a subscription, membership, or fee for access.

1: [Margel D et al](#) Long-term intermittent exposu... [PMID: 14605040]

[Related Articles](#), [Links](#)

- LITERATURE:
 - Aggregators:
 - EBSCO
[*full-text online](#)
 - MD Consult LLC
[*full-text online](#)
 - Ovid Technologies, Inc.
[*full-text online](#)
 - ProQuest Information and Learning
[*full-text online](#) [*full-text PDF](#)
 - Libraries
 - Publishers/providers:
 - HighWire Press
[*full-text online](#)
- MEDICAL:
 - Consumer health:
 - MEDLINEplus Health Information
[Sleep Apnea](#)
- MOLECULAR BIOLOGY DATABASES:
 - Structure:
 - Hazardous Substances Data Bank
[CARBON DIOXIDE](#)



Part III

TOXLINE and Other Bibliographic Files



TOXLINE

TOXicology Literature onLine

- Covers pharmacological, biochemical, physiological, environmental, and toxicological effects of chemicals/other agents on living systems
- Citations, Abstracts, Keywords and/or MeSH (Medical Subject Headings)
- CAS Registry Numbers
- From 1965 to date (and earlier)
- Drawn from Secondary Sources, varying unit record formats
- Components – TOXLINE Core (on PubMed, accessible via TOXNET) and TOXLINE Special (on TOXNET)
- Over 3 million toxicology related records combined



TOXLINE Core (on PubMed)

- Toxicology Subset limit of MEDLINE on PubMed
- Similar to TOXLINE's former TOXBIB subfile
- Drawn from standard biomedical journal literature
- Accessible directly on PubMed or from the TOXLINE search screen on TOXNET
- Some features of PubMed:
 - MeSH Searching
 - Limit by field, publication type, age, gender, language, human or animal, etc.
 - Cubby – to store and update searches
 - Related articles
 - LinkOut + Links to Books
 - Interlibrary Loan (Loansome Doc)



TOXLINE Special (on TOXNET)

- Technical Reports and Research projects
 - Federal Research in Progress (FEDRIP)
 - Toxicology Document and Data Depository (NTIS)
 - Toxicology Research Projects (CRISP)
 - Toxic Substances Control Act Test Submissions (TSCATS)

- Special Journal and Other Research Literature
 - Developmental and Reproductive Toxicology (DART)
 - International Labour Office (CIS)
 - Swedish National Chemicals Inspectorate (RISKLINE)



TOXLINE Special (continued)

- Archival Collections (No Longer Being Updated)
 - Aneuploidy (ANEUPL)
 - Environmental Mutagen Information Center file (EMIC)
 - Environmental Teratology Information Center file (ETIC)
 - Epidemiology Information System (EPIDEM)
 - Hazardous Materials Technical Center (HMTC)
 - International Pharmaceutical Abstracts (IPA)
 - NIOSHTIC (NIOSH)
 - Pesticides Abstracts (PESTAB)
 - Poisonous Plants Bibliography (PPIB)
 - Toxicological Aspects of Environmental Health (BIOSIS)



TOXLINE Special (continued)

- Some Features of TOXLINE Special
 - Relevancy Ranking
 - Toggle between TOXLINE Special and TOXLINE Core
 - Automatic Mapping to MeSH terms
 - Link to TOXLINE Special from *ChemIDplus*
 - Related Articles

Note: Search algorithms and display formats of TOXLINE Special and TOXLINE Core vary.



Another Toxicology Literature File

Developmental and Reproductive Toxicology (DART/ETIC)

101,812 Records

- Covers Developmental and Reproductive Toxicology (including Teratology)
- Components – DART Core (on PubMed) and DART Special (on TOXNET)



Search Page - Toxicology Literature Files

- One Box Search for:
 - Chemicals – enter chemical names or CAS Registry numbers.
Let system add synonyms (default) or use exact terms entered.
 - Other Terms
- Select TOXLINE Special, TOXLINE Core or both (default)
- Browse Index for:
 - All Words
 - Authors
 - MeSH Headings/Keywords
 - CAS Registry Numbers
- Automatic Term Mapping to MeSH & UMLS
 - e.g. passive smoking --- tobacco smoke pollution
- Limits
 - For more precise searching – to search within all fields, title only, author only, by specific range of years of publication, subfile, language, etc.



Search Results Page - Toxicology Literature Files

- Displays title, author, source, subfile of retrieved records
- Relevancy Ranked Display
- Select Record(s) of Interest
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a new Basic Search – Returns you to Search Page with blank query box
- Or Search can be modified or begun anew directly on Results Page
- Sort Results – By year of publication, title, author, entry month, relevance, in ascending or descending order
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Brief, Full, Abstract, Tagged
- Browse Index
- Return to TOXNET Home



Selected Record Page - Toxicology Literature Files

- Displays full bibliographic record – Title, Author, Source, Abstract, keywords, etc.
- Search Terms **highlighted in Red**
- Hot Linked Items (e.g. authors, keywords, CAS registry numbers) highlighted and underlined in Blue
- Related Records
- Return to Search Results page
- Download – Brief, Full, Abstract, Tagged
- Modify Search – Returns you to Search Screen with query intact
- Begin a new Basic Search – Returns you to search Screen with blank query box
- Or Search can be modified or begun anew directly on Results Page
- View Details of Search Strategy
- View Search History and combine search statements
- Browse Index
- Return to TOXNET Home



Toxicology Bibliographic Information

[Tox. & Env. Health](#) [TOXNET](#) [TOXLINE](#)

Databases

HSDB	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
Toxicology Bibliographic Info	i
DART/ETIC	i
TRI	i
ChemIDplus	i
TOXNET Home	

Search TOXLINE

brain cancer pesticides

Search

Clear

For chemicals, add synonyms
and CAS numbers to search:

Yes No

Search in

- TOXLINE Special
- TOXLINE Core on PubMed
- Both **New Default**

Limits

Browse the Index

Other NLM Resources

[Tox/Env. Health Home Page](#)
[Haz-Map](#)
[Tox Town](#)
[Household Products Database](#)
[ALTBIB](#)
[MEDLINEplus Tox/Env. Health](#)
[MEDLINE/PubMed](#)
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Support Pages

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**TOXLINE Special
Search Results**

- Save Checked Items
- Sort
- Details
- History
- Download
- Modify Search
- Basic Search
- Browse Index
- Help
- TOXNET Home

brain cancer pesticides

For chemicals, add synonyms and CAS numbers to search: Yes No

Items **1** through **20** of **57**

Pages: [1](#) [2](#) [3](#)

References are sorted in *relevancy ranked* order.

Click on **Sort** to change the order of the retrieved References.

Select Record	Reference
1 <input type="checkbox"/>	Pesticide Prioritization for a Brain Cancer Case-Control Study Sanderson WT ; Talaska G ; Zaebst D ; Davis-King K ; Calvert G Environmental Research, Vol. 74, No. 2, pages 133-144, 28 references, 1997 [NIOSH]
2 <input type="checkbox"/>	Pesticide prioritization for a brain cancer case-control study. SANDERSON WT ; TALASKA G ; ZAEBST D ; DAVIS-KING K ; CALVERT G ENVIRONMENTAL RESEARCH; 74 (2). 1997. 133-144. [BIOSIS]
3 <input type="checkbox"/>	Occupational Risk Factors for Brain Tumors among Women in Shanghai, China Heineman EF ; Gao Y-T ; Dosemeci M ; McLaughlin JK Journal of Occupational and Environmental Medicine, Vol. 37, No. 3, pages 288-293, 22 references, 1995 [NIOSH]
4 <input type="checkbox"/>	Brain cancer mortality among French farmers: The vineyard pesticide hypothesis. VIEL J-F ; CHALLIER B ; PITARD A ; POBEL D ARCHIVES OF ENVIRONMENTAL HEALTH; 53 (1). 1998. 65-70. [BIOSIS]
5 <input type="checkbox"/>	Family pesticide use and childhood brain cancer. DAVIS JR ; BROWNSON RC ; GARCIA R ; BENTZ BJ ; TURNER A ARCH ENVIRON CONTAM TOXICOL; 24 (1). 1993. 87-92. [BIOSIS]



[Related Records](#)

[Search Results](#)

[Download](#)

[Basic Search](#)

[Browse Index](#)

[Modify Search](#)

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[TOXNET Home](#)

brain cancer pesticides

For chemicals, add synonyms and CAS numbers to search: Yes No

Item 1 of 57

Pesticide Prioritization for a Brain Cancer Case-Control Study

Authors:

[Sanderson WT](#)
[Talaska G](#)
[Zaebst D](#)
[Davis-King K](#)
[Calvert G](#)

Source: Environmental Research, Vol. 74, No. 2, pages 133-144, 28 references, 1997

Abstract:

Procedures used to select **pesticides** to be included in a NIOSH case control study examining the risk of **brain cancer** in farm workers in Iowa, Michigan, Minnesota, and Wisconsin associated with **pesticide** use and other environmental exposures was discussed. A procedure to identify and prioritize the **pesticides** most appropriate for the study was needed because of the large number and variety of **pesticides** available, approximately 24,000 commercially registered **pesticides**, therefore making it impossible to investigate them all. Lists of **pesticides** were created to document those used in the four states and in the US as a whole utilizing data from the US Department of Agriculture and the departments of agriculture and land grant colleges in each state. **Pesticides** were then prioritized according to the criteria: volume of use before 1985, ranking of use in the four states and the US as a whole according to **pesticide** type, and toxicologic evidence of carcinogenic, teratogenic, and mutagenic effects. The criterion '**pesticide** use before 1985' was chosen to allow a latency period of at least 10 years for **brain cancer**. The study was to be based on **brain cancer** cases diagnosed in the four states from 1985 on. A total of 240 **pesticides** were used in the four states: 102 herbicides, 81 insecticides, 32 fumigants, and 35 fungicides. Using the criteria above, the list was reduced to 56 herbicides, 49 insecticides, 17 fumigants, and 12 fungicides. The final list represented more than 99% of the total pounds of herbicides and insecticides and more than 98% of the total pounds of fungicides and fumigants used in the states before 1985. Lists of the priority **pesticides** are to be sent to the study participants before the study questionnaire is administered to allow them time to recall details of their including specific years of use and crops they were used on. The authors conclude that the procedures used to select the **pesticides** to be examined in this study are useful for documenting past **pesticide** use.

Keywords:

DCN-241835
NIOSH Author
Agricultural chemicals
Occupational exposure
Epidemiology
Brain tumors
Risk analysis
Information systems
Agricultural workers

Coden:


ENVRAL



Entry Month: October, 1998

Year of Publication: 1997

Secondary Source ID: NIOSH/00241410

LIMITS

 **National Library of Medicine**
Specialized Information Services

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Toxicology Bibliographic Information [Tox. & Env. Health](#) [TOXNET](#) [TOXLINE](#) [Limits](#)

Databases **Search TOXLINE**

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GENE-TOX	i
CCRIS	i
Multi-Databases	i
Toxicology Bibliographic Info	i
DART/ETIC	i
TRI	i
ChemIDplus	i
TOXNET Home	

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- [MEDLINE/PubMed](#)
- [DIRLINE](#)
- [NLM Gateway](#)

Support Pages

- [Help](#)
- [Fact Sheet](#)
- [Sample Record](#)

beryllium workers

Add chemical synonyms and CAS numbers to search:
 Yes No

Search in: TOXLINE Special TOXLINE Core on PubMed Both **New Default**

Search fields: All fields Titles Authors (e.g., Smith H)

Search: exact words singular & plural forms word variants
Search records with: the phrase all words any words

25000 Maximum records returned
Year of Publication: 2000 through 2004
Only search documents added in the last months.

TOXLINE Components: All, ANEUP, BIOSIS, CIS, CRISP, DART

Language: All, English, Afrikaans, Arabic, Armenian, Azerbaijani

To select more than one component, click while holding the CTRL (PC) or CMD (Mac) key.



TOXLINE Special Search Results

▶ [Tox. & Env. Health](#) ▶ [TOXNET](#) ▶ [TOXLINE Special](#)

Save Checked Items

Sort

Details

History

Download

Modify Search

Basic Search

Browse Index

Help

TOXNET Home

beryllium workers

Search Clear Limits

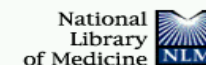
For chemicals, add synonyms and CAS numbers to search: Yes No

Items 1 through 3 of 3

References are sorted in [relevancy ranked](#) order.

Click on **Sort** to change the order of the retrieved References.

Select Record	Reference
1 <input type="checkbox"/>	CHRONIC BERYLLIUM DISEASE AMONG BERYLLIUM EXPOSED WORKERS ROSSMAN M Crisp Data Base National Institutes of Health [CRISP]
2 <input type="checkbox"/>	CHRONIC BERYLLIUM DISEASE AMONG BERYLLIUM EXPOSED WORKERS ROSSMAN M Crisp Data Base National
3 <input type="checkbox"/>	Lung cancer case-control study of beryllium workers. Sanderson WT; Ward EM; American Journal of Industrial Hygiene Association [AJIH]



Entrez PubMed Nucleotide Protein Genome Structure OMIM PMC Journals Books

Search PubMed for beryllium[TI] workers[TI] AND 2000:2004[dp] AN Go Clear

Limits Preview/Index History Clipboard Details

Display Summary Show: 20 Sort Send to Text

Items 1-5 of 5 One page.

- 1:** [Homg CJ, Homg PH, Lin SC, Tsai JL, Lin SR, Tzeng CC.](#) [Related Articles, Links](#)
Determination of urinary beryllium, arsenic, and selenium in steel production workers. *Biol Trace Elem Res.* 2002 Sep;88(3):235-46.
PMID: 12350133 [PubMed - indexed for MEDLINE]
- 2:** [Deubner DC, Lockey JL, Kotin P, Powers MB, Miller F, Rogers AE, Trichopoulos D.](#) [Related Articles, Links](#)
Re: Lung cancer case-control study of beryllium workers. Sanderson WT, Ward EM, Steenland K, Petersen MR. *Am J Ind Med.* 2001. 39:133-144.
Am J Ind Med. 2001 Sep;40(3):284-8. No abstract available.
PMID: 11598976 [PubMed - indexed for MEDLINE]
- 3:** [Henneberger PK, Cumro D, Deubner DD, Kent MS, McCawley M, Kreiss K.](#) [Related Articles, Links](#)
Beryllium sensitization and disease among long-term and short-term workers in a beryllium ceramics plant.
Int Arch Occup Environ Health. 2001 Apr;74(3):167-76.
PMID: 11355290 [PubMed - indexed for MEDLINE]

About Entrez

Text Version

Entrez PubMed

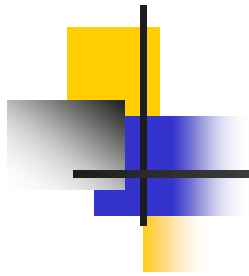
Overview
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New/Noteworthy
E-Utilities

PubMed Services

Journals Database
MeSH Database
Single Citation
Matcher
Batch Citation Matcher
Clinical Queries
LinkOut
Cubby

Related Resources

Order Documents



Part IV

TRI, Specialty Files, New Initiatives



Toxics Release Inventory (TRI) U.S. Environmental Protection Agency (EPA)

TRI 95-01 – 577,790 Records
(Coming soon TRI87-02)

- Facility Identification (Facility Name, Address, Phone, etc.)
- Substance Identification (Chemical Name, CAS RN, Uses, etc.)
- Environmental Release of Chemical (in Air, Water, Land, Underground Injection)
- Waste Treatment
- Off-Site Waste Treatment
- Source Reduction and Recycling (Quantity Released, Energy Recovery, Quantity Recycled, Quantity Treated)



TRI Background

- Right-to-Know Movement – Workplace, Community
- OSHA Hazard Communication Standard – 1983
- SUPERFUND = CERCLA (1980)
- Bhopal (1984) and smaller scale chemical disasters
- SARA (Superfund Amendments and Reauthorization Act) (1986)
 - Title 3 = Emergency Planning and Community Right-to-Know Act
 - Section 313 = Toxic Release Reporting
- Pollution Prevention Act of 1990



Search Page - TRI

- Several search query boxes – fill in any combination.
- Chemical names or CAS Registry numbers. Let system add synonyms (default) or use exact terms entered.
- Select Year(s) – 1995-2001
- Facility Name(s)
- Facility Location (state, city/state, county/state, zip)
- Ranging
 - Greater than _____ pounds
 - Total Release, Air, Water, Land, Underground Injection
 - Or “No Release Selected”
- Browse Index for:
 - All Words
 - Chemical Name
 - CAS Registry Number
 - Facility Name
 - Facility City



Search Results Page - TRI

- Displays facility name, chemical, city/state of retrieved records.
- Unsorted order
- Select Record(s) of Interest
- Calculate Releases – Tabular Display of Total Environmental Releases and Off-Site Waste Transfers for all retrieved records.
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a new Basic Search – Returns you to Search Page with blank query box (note: search screen can't be modified directly from this page)
- Sort Results – By substance name, facility name, city, or state. Ascending or Descending.
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Brief or Full Format
- Browse Index
- Get Help
- Return to TOXNET Home



Selected Record Page - TRI

- Full record displayed
- Choose fields for display from Contents (expand, contract categories)
- Navigate – Next Item, Previous Item
- View Details of Search Strategy
- Modify Search – Returns you to Search Screen with query intact
- Begin a New Search – Returns you to Search Screen with blank query box
- Browse Index
- Get Help
- Download – In Full Format
- Return to TOXNET Home
- Link to records for the same chemical in Other Files - (including TOXLINE and ChemID*plus*)



Toxics Release Inventory

[Tox. & Env. Health](#) [TOXNET](#) [TRI](#)

Databases

HSDB	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
Toxics Release Inventory	i
ChemIDplus	i
TOXNET Home	

Search TRI

Chemical Name or CAS Registry Number

Add synonyms and CAS numbers to search:

Yes No

TRI Files:

2001 2000 1999 1998
 1997 1996 1995

Facility Names

(Separate multiple entries with commas)

Facility Location

(Separate multiple entries for state, city/state, or zip with commas. For example: NJ, DE, or Trenton NJ, Houston TX, or 21113, 21224.)

State City/State
 County/State Zip

Greater Than for

Other NLM Resources

- [Tox/Env. Health Home Page](#)
- [Haz-Map](#)
- [Tox Town](#)
- [Household Products Database](#)
- [ALTBIB](#)
- [MEDLINEplus Tox/Env. Health](#)
- [MEDLINE/PubMed](#)
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TRI2001, TRI99 Search
Results

[Tox. & Env. Health](#) [TOXNET](#) [TRI2001, TRI99](#)

Calculate Release!

Save Checked Items

Sort

Details

History

Download

Modify Search

New Search

Browse Index

Help

TOXNET Home

Please click on **Modify Search** button to modify TRI search strategy.

[TRI2001](#): 2 [TRI99](#): 2

Click on the database name to repeat the search in that database

Items 1 through 4 of 4

Facility/Substance Names are *unsorted*.

Select Record	Database	Facility/Substance Name
1 <input type="checkbox"/>	TRI2001	YORK CASKET-MISSOURI METHYL ETHYL KETONE MARSHFIELD, MO
2 <input type="checkbox"/>	TRI2001	WILCORP INDS. INC. - MAR METHYL ETHYL KETONE MARSHFIELD, MO
3 <input type="checkbox"/>	TRI99	WILCORP INDS. INC. METHYL ETHYL KETONE MARSHFIELD, MO
4 <input type="checkbox"/>	TRI99	YORK CASKET-MISSOURI METHYL ETHYL KETONE MARSHFIELD, MO

Contents

Contract all categories

Expand all categories

Select

Clear

- [FULL RECORD](#)
- [Facility Identification](#)
- [Substance Identification](#)
- [Environmental Release of Chemical](#)
- [Waste Treatment](#)
- [Off-Site Waste Transfer](#)
- [Source Reduction and Recycling](#)
- [Administrative Information](#)

TRI99
METHYL ETHYL KETONE
YORK CASKET-MISSOURI
MARSHFIELD, MO

For other data, click on the Table of Contents

Environmental Release of Chemical:

Non-Point Air Emissions Estimates:

Non-Point Air Release: 1,900 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Point Air Emissions Estimates:

Point Air Release: 17,000 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Total Air Release: 18,900 lbs./rep yr. 1999

Water Discharge Estimates:

Receiving Stream: NA

Water Release: NA

Basis of Estimate: 0%

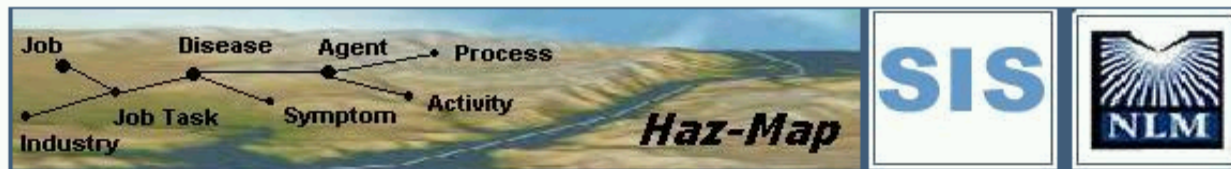
Total Water Release: 0 lbs./rep yr. 1999

Underground Injection Total: 0 lbs./rep yr. 1999

Land Release Estimates:

Disposal Method: (D03) Land Treatment/Application/Farming

Land Release: NA



Search as     Text Search

[Haz-Map Search](#) [More Searches](#) [Haz-Map Help](#) [Glossary](#) [References](#)

Browse Haz-Map

- **Hazardous Agents**
 1. [By Types of Agents](#)
 2. [By Adverse Effects](#)
 3. [Alphabetically](#)

- **Occupational Diseases**
 1. [By Types of Diseases](#)
 2. [By **J**obs and **S**ymptoms](#)
 3. [Alphabetically](#)

- **High Risk Jobs**
 1. [By Types of Jobs](#)
 2. [Alphabetically](#)

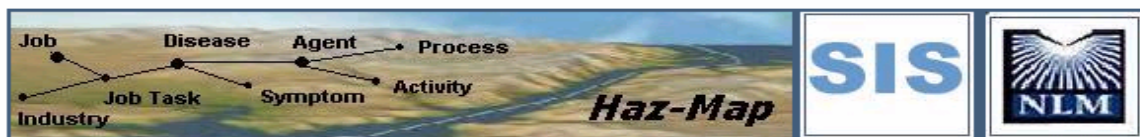
Haz-Map: Information on Hazardous Chemicals and Occupational Diseases

by

Jay A. Brown, M.D., M.P.H.

[Haz-Map Fact Sheet](#) | [Download Haz-Map Brochure](#)

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Last updated: February 14, 2003



Search

as



Highlight Term(s) First

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[More Searches](#)

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[Browse Haz-Map by Jobs](#)

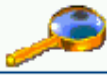
[Search TOXNET](#)

Information about this job:

Carpenters

- **High risk job tasks associated with this job:**
 - Apply arsenic preservatives to wood
 - Contaminate skin or inhale spray while using pentachlorophenol
 - Handle agents that cause allergic contact dermatitis or contact urticaria
 - Installed insulation before 1975
 - Machine allergenic wood and inhale dust
 - Remove insulation installed before 1975
 - Saw or sand arsenic-treated wood
 - Saw or sand creosote-treated wood
 - Use epoxy, isocyanate, or formaldehyde-resin adhesives, finishes, or sealants
 - Use n-hexane as a solvent in glues, coatings, or degreasers
 - Work with glue solvents



Search as  Agent  Disease  Job  Text Search

[Haz-Map Search](#) [More Searches](#) [Haz-Map Help](#) [Glossary](#) [References](#)

[Browse Haz-Map](#)

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Agent Name	n-Hexane
Alternative Name	Hexane
CAS Number	110-54-3
Formula	C6-H14
Major Category	Solvents
Synonyms	Hexyl hydride, normal-Hexane
Category	Alkanes (Paraffins)
Description	Colorless liquid with a gasoline-like odor;
Sources/Uses	Used as a solvent, especially in the adhesive and shoe industries; abused by glue sniffers for its euphoric effects; [LaDou, p. 371] Used in shoe and furniture manufacture to dissolve glue; also used in adhesive tape manufacturing; [Sullivan, p. 1124]
Comments	n-Hexane is in the list of "Some volatile substances which may be abused by inhalation" published on the web site of the U.N. International Drug Control Programme, indicating its potential to cause narcosis in workers. In addition to CNS solvent syndrome, n-Hexane can cause motor neuropathy.

Exposure Assessment	
<u>BEI</u>	2,5-Hexanedione in urine = 5 mg/g creatinine; end of shift; screen for n-hexane in end-expired air; ACGIH Notice of Intended Change (2001): 2,5-Hexanedione (free) in urine = 4 mg/L end of shift near end of workweek;
<u>Skin Designation (ACGIH)</u>	Yes
<u>TLV (ACGIH)</u>	50 ppm
<u>PEL (OSHA)</u>	500 ppm
<u>IDLH (NIOSH)</u>	1100 ppm
<u>Excerpts from Documentation for IDLHs</u>	It has been reported that a 10-minute exposure to 5,000 ppm caused dizziness and a sensation of giddiness.
<u>Vapor Pressure</u>	124 mm Hg
<u>Odor Threshold Low</u>	65 ppm
<u>Odor Threshold High</u>	248 ppm
<u>Explanatory Notes</u>	IDLH = 10% of LEL (lower explosive limit); Odor threshold from AIHA;
<u>MAK</u>	50 ppm
<u>Half Life</u>	Urine (2,5-hexanedione): 15 hours; blood: 2-3 hours; fat: 64 hours; [TDR, p. 1480]
<u>Reference Link</u>	ATSDR ToxFAQs - n-Hexane
<u>Flammability (NFPA)</u>	3: may ignite at ambient temperature
Adverse Effects	
<u>Neurotoxin</u>	Motor Neuropathy

Household Products Database

National Institutes of Health
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Ingredients

MSDS

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Health & Safety Information on Household Products

What's under your kitchen sink, in your garage, in your bathroom, and on the shelves in your laundry room? Do these household products pose a potential health risk to you and your family?

Find out what's in these products and what are the potential health effects, and other safety and handling information. [Find a product...](#)

For advice if someone's poisoned, call your local [Poison Center](#) at (1-800-222-1222).



Household Products Database

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Auto Products

Brake Fluid, De-icer, Defogger,
Lubricant, Sealant, and more...



Home Inside

Air Freshener, Bleach,
Detergent, Toilet Bowl Cleaner,
and more...

Pesticides

Animal Repellent, Fungicide,
Herbicide, Insecticide,
and more...



Landscape / Yard

Fertilizer, Lawn Care,
Swimming Pool Products,
and more...



Personal Care / Use

Antiperspirant, Hair Spray,
Makeup, Shampoo, Soap,
and more...



Home Maintenance

Caulk, Grout, Insulation,
Paint, Putty, Stain, and more...

Hobbies & Crafts

Adhesive, Glaze, Primer,
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Brand Information

Brand Name: Kilz Kwik-Start Water-Based Primer Sealer

Form: liquid

Product Category: Home maintenance

Purpose: Primer

Type: latex

Customer Service No.: 800-325-3552

Date Entered: 2001-06-14

Related Items: [Products with similar usage in this database](#)

Manufacturer

Manufacturer: Masterchem Industries, Inc.

Address: PO Box 368

City: Barnhart

State: MO

Zip Code: 63012

Telephone Number: 636-942-2510

Fax Number: 636-942-3663

Toll Free Number: 800-325-3552

Date Info Verified: 2003-01-01

Related Items: [Products by this manufacturer](#)

Health Effects

Search TOXNET

Warning from Label: CAUTION: USE ONLY WITH ADEQUATE VENTILATION.

Harmful if swallowed. Avoid contact with eyes. May cause eye, nose and throat irritation. Avoid breathing of dust, vapors and spray mist. Open windows and doors or use other means to ensure fresh air entry during application and drying. If you experience eye watering, headaches, or dizziness, increase fresh air or leave area. Close container after each use. Wash thoroughly after handling, and before smoking and eating. **WARNING:** This product contains chemicals known to the state of California to cause cancer and birth defects, or other reproductive harm. Keep out of reach of children.

Acute Health Effects: From MSDS:

EFFECTS OF OVEREXPOSURE:

Inhalation: May cause irritation to upper respiratory tract. Shortness of breath and dizziness.

Splash (Eyes): Can cause irritation, burning and redness.

Splash (Skin): Prolonged or repeated contact may cause irritation.

Ingestion: Gastrointestinal distress, vomiting and diarrhea.

PRIMARY ROUTE(S) OF ENTRY: DERMAL, INHALATION, INGESTION

Chronic Health Effects: MSDS: Splash (Skin): Prolonged or repeated contact may cause irritation.

Carcinogenicity: MSDS: None of the ingredients in this product is listed as a carcinogen.

First Aid: MSDS: EMERGENCY AND FIRST AID PROCEDURES: Inhalation: Remove to fresh air. Restore breathing. Treat symptomatically. Consult a physician. Splash (eyes): Flush immediately with large amounts of water for at least 15 minutes. Take to physician for medical treatment. Splash (skin): Wash affected areas with soap and water. Remove contaminated clothing. Consult a physician if irritation persists. Ingestion: Drink 1 or 2 glasses of water to dilute. DO NOT induce vomiting. Consult physician or poison control center immediately. Treat symptomatically.

Health Rating: 2

Flammability Rating: 0

Reactivity Rating: 0

HMIS Rating Scale: 0 = Minimal; 1 = Slight; 2 = Moderate; 3 = Serious; 4 = Severe;
N = No information provided by manufacturer; * = Chronic Health Hazard

MSDS Date: 2000-09-26

Handling/Disposal

Handling: MSDS: PRECAUTIONS TO BE TAKEN IN HANDLING AND STORING: Store in accordance with OSHA 1910.106. Store in well ventilated areas. Protect from freezing. Frozen product may coagulate and become unusable.

OTHER PRECAUTIONS: DO NOT TAKE INTERNALLY. Avoid prolonged contact with skin. Keep closure tight and container upright to prevent leakage. Do not store near heat, sparks, or open flame. Do not breathe spray. Containers must not be washed out or used for other purposes. Avoid contact with or breathing of vapors released during curing process. Do not remove or deface container label. Keep out of the reach of children.

Disposal: MSDS: WASTE DISPOSAL METHOD: Dispose of in accordance with all local, state and federal regulations. Dry product and empty containers may be landfilled. Full or partially full containers should be dried or coagulated with the liquid portion poured off. Coagulated material should be dried before landfilling. Product may also be incinerated.

Ingredients from MSDS/Label

Chemical	CAS No / Unique ID	Percent
Talc (non-fibrous)	014807-96-6	5-10
Calcium carbonate	001317-65-3	5-10
Titanium dioxide	013463-67-7	5-10
Ethylene glycol	000107-21-1	2.62
Water	007732-18-5	30-40
Acrylic polymer/copolymer	999999-63-1	25-40

Note: Brand names are trademarks of their respective holders.
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Enter country name or other term(s):

Or click on map below:



Select a country

Select an organization



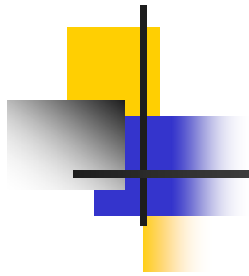
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More to Come

- Drugs and Lactation
- Endocrine Disruptors
- WISER - for PDA
- Toxicology Education Portal & ToxLearn
- ChemID Advanced Version



Part V

Non-NLM Resources



Professional Associations

- Society of Toxicology – <http://www.toxicology.org/>
- Society of Environmental Toxicology and Chemistry – <http://www.setac.org>
- American Academy of Clinical Toxicology – <http://www.clintox.org>
- American Association of Poison Control Centers – <http://www.aapcc.org>
- Society of Risk Analysis – <http://www.sra.org>
- Other groups in environmental health, occupational health, industrial hygiene, health physics etc.



U.S. Government Resources

- Agency for Toxic Substances and Disease Registry (ATSDR) – <http://www.atsdr.cdc.gov>

- Environmental Protection Agency (EPA) – <http://www.epa.gov>

- Food and Drug Administration – <http://www.fda.gov>
 - National Center for Toxicological Research – <http://www.fda.gov/nctr>

- National Institute for Occupational Safety and Health – <http://www.cdc.gov/niosh>



U.S. Government Resources (continued)

- National Institute of Environmental Health Sciences – <http://www.niehs.nih.gov>
- National Toxicology Program – <http://ntp-server.niehs.nih.gov>
- U.S. Chemical Safety and Hazard Investigation Board – <http://www.chemsafety.gov>

Some State Government Sites

- New Jersey Department of Health and Senior Services – Division of Epidemiology, Environmental and Occupational Health – <http://www.state.nj.us/health/eoh>
- California – Office of Environmental Health Hazard Assessment – <http://www.oehha.ca.gov>



Some Chemical Databases

- Chemfinder – <http://www.chemfinder.cambridgesoft.com>
- Scorecard (from Environmental Defense) – <http://www.scorecard.org>
- Environmental Fate Databases & more (from Syracuse Research Corporation) – http://www.syrres.com/esc/free_demos.htm
- EXTOXNET (pesticide information) – <http://ace.orst.edu/info/extoxnet>



Some Chemical Databases (continued)

- PAN (Pesticide Action Network) Pesticides Database – <http://www.pesticideinfo.org>
- Where to Find Material Safety Data Sheets on the Internet – <http://www.ilpi.com/msds>
- RxList, the Internet Drug Index – <http://www.rxlist.com>
- International Programme for Chemical Safety (IPCS) INCHEM – <http://www.inchem.org/>

Also Consider:

- Scirus - Elsevier Science - <http://www.scirus.com/>



Other Web Sites

- UNEP (United Nations Environment Programme) Chemicals – <http://www.chem.unep.ch>
- Intergovernmental Forum on Chemical Safety - <http://www.who.int/ifcs/>
- Inter-Organization Programme for the Sound Management of Chemicals - <http://www.who.int/iomc/>
- National Council for Science and the Environment – <http://www.cnie.org>
- Society of Environmental Journalists – <http://www.sej.org>
- TEHIP/NLM Web Links – <http://sis.nlm.nih.gov/Tox/ToxWebLinks.html>



Some Commercial (\$) Databases

- ARIEL Insight – Ariel Research – <http://www.arielresearch.com>
- BIOSIS Previews – BIOSIS – <http://www.biosis.org>
- Chemical Abstracts & CAS Registry – Chemical Abstracts Service – <http://www.cas.org> (also <http://stnweb.cas.org>)
- CCINFOweb (CHEMINDEX & IPCS/INCHEM are free) – CCOHS – <http://www.ccohs.ca>
- CIS Database (on occupational health) (from the International Labour Office) (free as a TOXLINE subfile) – <http://www.ilo.org/public/english/protection/safework/cis/products/cisdoc.htm>



Some Commercial (\$) Databases (continued)

- EMBASE – Elsevier Science – <http://www.embase.com>
- Environment Abstracts – Congressional Information Service – available from Dialog - <http://www.dialog.com/>
- MICROMEDEX Databases – MICROMEDEX – <http://www.micromedex.com>
- Science Direct - Elsevier - <http://www.sciencedirect.com/>
- Toxicology Abstracts – Cambridge Scientific Abstracts – <http://www.csa.com>
- Web of Science – ISI – <http://www.isinet.com/>



Some Web Search Engines and Tools

- AltaVista – <http://www.altavista.com>
- Google – <http://www.google.com>
- Hotbot – <http://www.hotbot.com>
- Yahoo – <http://www.yahoo.com>
- Meta Search Engines
 - Go2Net – <http://www.go2net.com>
 - Dogpile – <http://www.dogpile.com>
 - Ask Jeeves – <http://www.ask.com>
- Searchenginewatch – <http://www.searchenginewatch.com>
- Mailing List Directories – CATALIST - <http://www.lsoft.com/lists/listref.html>

TOXNET Exercises

[Note: There is typically more than one “right” approach to answering each of the following questions. Answers, where they are provided, are merely representative, not definitive. Explore.]

TOXICOLOGY DATA FILES

1. What is the CAS registry number and octanol/water partition coefficient of 2,6-dinitrotoluene and what is this chemical used for? [HSDB]

In HSDB, search for **2,6-dinitrotoluene** and click on the 2,6-dinitrotoluene record on the Search Results Page. In the Table of Contents, expand **Chemical/Physical Properties** and click on **Octanol/Water Partition Coefficient**. Expand **Manufacturing/Use Information** and click on **Major Uses**.

2. Has 2,6-dinitrotoluene been shown to be mutagenic in the Ames salmonella test? [HSDB]

MODIFY above search to **2,6-dinitrotoluene ames**, and click on **2,6-dinitrotoluene** record.
Note: You may also wish to check other files, such as GENE-TOX and CCRIS.

3. What is the oral LD50 of caffeine in male rabbits? Also, click on **DETAILS** to view the search strategy. [HSDB]

Search for **oral ld50 caffeine male rabbits** and click on **caffeine** record.
Note: On target hit displays first.

4. Has caffeine been studied as a tumor promoter? Does it cause mutations? [CCRIS, GENE-TOX]

From HSDB caffeine record (above), click on **Other Files**. Select CCRIS. Expand Studies data in Table of Contents and check the boxes for **Tumor Promotion Studies** and **Mutagenicity Studies**. Return to HSDB. Click on **Other Files** again and select GENE-TOX. **Select Mutagenicity Studies**.

5. Which of the toxicology data files contain information on ammonia? What is the Inhalation Reference Concentration (RfC) of ammonia? (Note: the RfC is a non-carcinogenic risk assessment parameter) Also, view the DOWNLOAD options available. [Multi-Data Base and IRIS]

Select the **Multi-Database** option on the TOXNET main page. Search for **ammonia**. Click on the IRIS ammonia record. Expand **Chronic Health Hazard Assessment for Noncarcinogenic Effects** in Table of Contents. Click on **Reference Concentration for Chronic Inhalation Exposure (RfC)**.

TOXNET Exercises (continued)

6. What are some chemicals used in leather tanning and what are their human health effects? [HSDB]

Use the **limits** option of HSDB. Search for **leather tanning** in HSDB. Expand **Manufacturing/Use Information** and check the box for **Major Uses**. Click on several retrieved chemical records to view their “best sections” and click on **Human Health Effects** for these records in the Table of Contents.

7. Does nitrobenzene have any effect on sperm? Find some recent general articles on nitrobenzene. [HSDB, TOXLINE Core]

Search for **nitrobenzene sperm** in HSDB. Click on nitrobenzene record and view **Best Sections**. Click on **Other Files and** click on **TOXLINE Core**.

8. How does the U.S. Environmental Protection Agency characterize the carcinogenicity of methylmercury? [IRIS]

Search for **methylmercury** in IRIS and select the methylmercury record on the Search Results page. Expand category **II. Carcinogenicity Assessment for Lifetime Exposure**. Click on **II.A. Evidence for Human Carcinogenicity**.

9. Find any information on the occurrence or effects of methyl parathion in soil. Search using the chemical’s CAS Registry Number – 298-00-0. [HSDB]

Search HSDB for **298-00-0 soil** in the query box and scan the **Best Sections** of the methyl parathion record.

10. How do the Dutch RIVM and the U.S. EPA compare in their non-cancer oral risk values for chloroform? [ITER]

Search for **chloroform**. View **Risk Data: Non-Cancer Oral Table**.

11. Use Boolean operators and phrase searching to look for information on lung cancer or bladder cancer in workers, in HSDB.

Enter – (“**lung cancer**” [htox] OR “**bladder cancer**” [htox]) AND worker

TOXNET Exercises (continued)

TOXICOLOGY LITERATURE FILES

1. Search TOXLINE Special for articles by C.N. Pope. Sort retrieval by primary author names. [TOXLINE Special]

Search for “pope cn” in query box. On “Search Results” page, click on “SORT” button and sort by author.

2. Search TOXLINE Special and TOXLINE Core for phosphoric acid. Explore navigating through your retrieval, examining individual records, and going to linked records. [TOXLINE Special & Core]

Search for **phosphoric acid** in query box. Click on **Details** buttons in both databases to view the respective search strategies. Navigate the pages. Click on records of interest and on hot-linked data – e.g. keywords, author names, CAS registry numbers. Check for related records.

3. Find articles focused on the effects of diet on breast cancer. [TOXLINE Special & Core]

Try a **Limits** search. Enter **diet breast cancer** in the query box. Limit to **Titles**. Select **Both** TOXLINE Special and TOXLINE Core.

4. Find journal references on the treatment of arthritis by the anti-inflammatory agent Celebrex. [TOXLINE Core]

Search for **arthritis celebrex** in the query box. Select the TOXLINE Core radio button.

5. Use the EMIC subfile to determine whether peppermint been tested for mutagenicity. Check for English language articles. [TOXLINE Special]

Conduct a Limits search. Select EMIC as a TOXLINE Component and English as a language from the drop down menus. Enter **peppermint** in the query box.

6. Find information on the effects of alcohol on the fetus. [DART Special and DART Core]

Select **Both** DART Special and DART CORE. Search for **alcohol fetus** in the query box.

TOXNET Exercises (continued)

7. Search TOXLINE Core directly on PubMed to find articles on toxicological aspects of jellyfish. Search for articles published from 2000-2003 in English. [TOXLINE Core via PubMed directly].

Go to PubMed at <http://pubmed.gov>. Click on **Limits**. Enter **jellyfish** in the search query box. Limit the search to the toxicology subfile, the publication dates to 2000-2004 and the language to English.

8. Find information on renal failure associated with amanita mushroom poisoning. Look for English language articles published from 1995 to 2004. [TOXLINE Special]

Conduct a Limits search. Enter **amanita renal failure** in the query box. Restrict publication years to 1995-2003. Select English from the dropdown menu.

9. Use the HISTORY feature to look for hospital or medical waste incineration in TOXLINE Special. [TOXLINE Special]

First search for **“hospital waste” incinerat***. (Using quotes looks for the terms together as a phrase. The asterisk is for truncation and searches for words such as incinerate, incineration, etc.) Then search for **“medical waste” incinerat***. Press the HISTORY button and combine your two searches according to the instructions, and using an “OR” operator.

TOXIC CHEMICAL RELEASES

1. How much ammonia was released to the air and water in Milwaukee in 1999?

In TRI99, search for **ammonia** in the “chemical name” query box and for **Milwaukee/WI** in the “facility location (city/state)” query box. Click on “Calculate Releases.”

2. How much of the above releases came from Red Star Yeast and in what body of water did this facility discharge ammonia?

After above search, go back to the “TRI Search Results” screen. Click on the Red Star Yeast record. Click on “Environmental Release of Chemical” in the Table of Contents. Scroll down to “Water Discharge Estimates.”

TOXNET Exercises (continued)

3. What chemicals have been released to the air, in amounts greater than 100,000 pounds, over Old Hickory, Tennessee in 1995 and 1996? By what companies?

Search for **Old Hickory Tennessee** in the “facility location (city/state)” query box. Select **greater than 100,000 pounds** for “total air release.” Results page will display chemicals and companies.

4. Did Hewlett-Packard’s Newark, California facility transfer any 1,2,4-trichlorobenzene off-site for treatment in 1996? How much? Where to?

In TRI96, search for **1,2,4-trichlorobenzene** in the “chemical” query box, **hewlett-packard** in the “facility name” query box, and **newark california** in the “facility location (city/state)” query box. Click on “Off-Site Waste Transfer” in the Table of Contents.

5. What company has reported the highest underground injection release of a single chemical in 1999? What was the chemical?

In TRI99, select **10,000,000** and “Total Underground Injection” in the “Greater than ___ for ___” drop down menus. For the records retrieved, expand the “Environmental Release of Chemical” category. Click on “Underground Injection Total” for these records and compare the numbers. Identify the chemical with the highest number.

6. How many individual TRI98 reports have been filed on barium compounds?

In TRI98, search **barium compounds** in the chemical query box. Note the number of records retrieved listed at the top of the Search Results page.

TOXNET Exercises (continued)

HAZ-MAP

1. What are some high risk tasks associated with the job of carpet installation?
Click on **High Risk Jobs** and then on “Alphabetically.” Choose the letter “C” and click on **Carpet Installers**.
2. What are some hazards associated with the use of cobalt in the workplace?
Enter **Cobalt** in query box and click on “agent.” Click on **Cobalt**. Click on **Cobalt** again to view potential hazards. For Extra Credit – highlight a term or phrase (e.g. “cobalt chloride skin allergy” and search **TOXLINE**.
3. What are some hazards of leather tanning?
Perform a “text search” for **leather tanning** in the search query box. Click on first **leather tanning and finishing** as an Industry and then go back and click on **tanning leather** as a Process.

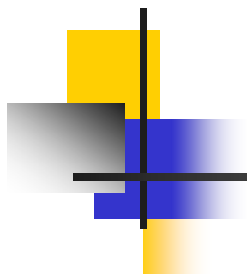
HOUSEHOLD PRODUCTS DATABASE

1. What is in Windex and are there any health dangers associated with it?
Enter **Windex** in query box. Click on your choice of Windex cleaner. View ingredient and health effects information.
2. Compare the toxicities of various pesticides used to treat ants.
Choose “Browse by Categories.” Click on **Pesticides**, then on **Insecticides** as a Category and **Ant** as a type. View the data on the various products.
3. What stick deodorants include the antibacterial ingredient triclosan?
Click on Ingredients. Enter **triclosan** in query box. Click on triclosan. Scan list of products.

TOXNET Exercises (continued)

WORLD WIDE WEB

1. Explore EPA's voluminous Web site, particularly the **Databases and Software** section located by clicking on their home page's **Information Sources**. Locate IRIS, ECOTOX, the Toxics Release Inventory, and the Safe Drinking Water Information System. Use the Advanced Search box to find documents with **mercury** in the title. [www.epa.gov]
2. Locate a full-text article about the ban on ephedra in the March-April 2004 issue of the **FDA Consumer** magazine. [www.fda.gov]
3. What chemicals are on the list of "Known to be Human Carcinogens" in the National Toxicology Program's Year 2002 10th Report of Carcinogens? [ntp-server.niehs.nih.gov]
4. Find the Agency for Toxic Substances and Disease Registry's TOXFAQ profile on nickel. [www.atsdr.cdc.gov]
5. Check out the National Council for Science and the Environment's Web site and find recent Congressional Research Service (CRS) reports, under their National Library for the Environment section, on **pesticides**. [www.cnie.org]
6. Which Florida universities offer graduate programs in toxicology? Check the Society of Toxicology's Resource Guide to Careers in Toxicology (under Public Outreach/Career Resources) [www.toxicology.org]
7. Explore the variety of data sources containing information on acrylonitrile, by searching ChemFinder. [www.chemfinder.com]
8. Where and on what dates will the fourth Society of Environmental Toxicology and Chemistry's World Congress be held? [www.setac.org]
9. What is New Jersey's rank among states in total release hazardous air pollutants? Use Scorecard (from Environmental Defense). Start by clicking on Pollution Rankings. [www.scorecard.org]
10. Use the BIOLOG file (one of Syracuse Research Corporation's Environmental Fate Data Bases – EFDB) to find information about DDT in sewage. [esc.syrres.com/esc/efdb.com]
11. Use the Environmental Journalism site to determine what environmental meetings will be coming up in October 2004. [www.nsej.org]
12. What are some common side effects of the drug Vioxx? Consult MedlinePlus' Drug Information page (data from the USP). [www.nlm.nih.gov/medlineplus/druginformation.html]
13. Who makes Kill Zone Flea and Tick Killer 2000? What are its active ingredients? How have various governmental agencies rated the carcinogenic potential of these ingredients? [www.pesticideinfo.org]
14. How many poison control centers in Texas are certified by the American Association of Poison Control Centers (AAPCC)? What are their addresses? The AAPCC's Poison Center Lists includes a list of certified centers. Find the nation-wide toll-free poisoning emergency phone number. [www.aapcc.org]



Part VI

ChemID*plus*



ChemID*plus*

- Chemical Identification File
- Chemical Dictionary/Directory File for chemicals cited in MEDLARS Files & outside resources
- Contains over 368,000 chemical records
- Structural Data for over 206,000 records
- Direct Link/Searches of MEDLINE, TOXNET, and other resources



ChemID*plus* Content

Names and Synonyms

- **Name of Substance**: Usually the most commonly used name, includes MeSH heading and USAN name
- **MeSH Heading**: NLM Medical Subject Heading
- **Systematic Name**: Describes molecular structure
- **Synonyms**: All other names found for the substance
- **Mixture Name**: Name of multi-component substance, one of which is the retrieved substance
- **SUPERLIST names**: The name used by regulatory/guidance lists



ChemID*plus* Content

- **CAS Registry Number**: Unique number of up to 9 digits assigned by Chemical Abstracts Service used to index chemicals. ChemIDplus uses the hyphenated format
- **ID**: The ID number is the CAS Registry Number in a non-hyphenated fixed length format or a unique number for entries that have no CAS Registry or NLM assigned numbers
- **Molecular Structure**: Display of structure (if present) via Chime or ChemSymphony
- **Registry Numbers**: All CAS Registry Numbers known to be assigned over time to a specific compound



ChemID*plus* Content

- **Formulas**: The molecular formula in a hyphenated format.
- **Classification Codes**: Describe the general category assigned by a given source to a chemical based on toxicity, use and application, pharmacologic and/or therapeutic category, and status on certain chemical lists.
- **Notes**: A textual description of a compound's use and utility, often from MeSH controlled vocabulary.
- **Locators**: The names of NLM databases, and other major resources that have information about a given compound, usually hyperlinked.



ChemID*plus* Lite

- The Lite search page is available at <http://chem2.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- Lite version does not allow structure searching and thus needs no plug-ins or special display software
- Chemical structures are displayed as GIF images
- Right truncation ("starts with") is available by using the asterisk (*) at the end of a search term
- More advanced data and structure searching can be done at the main ChemID*plus* page <http://chem.sis.nlm.nih.gov/chemidplus/>
- Spell checker

ChemIDplus Lite



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SIS



ChemIDplus

[Tox. & Env. Health](#) [TOXNET](#) [ChemIDplus](#)

Databases

HSDB	i
IRIS	i
ITER	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
Chemical Synonyms, Structures and more	i
TOXNET Home	

Search ChemIDplus

Enter the name (e.g. formaldehyde)
or registry number (e.g. 50-00-0)
to search

[Advanced
ChemIDplus
Search](#)

Other NLM Resources

[Tox/Env. Health Home Page](#)
[Haz-Map](#)
[Tox Town](#)
[Household Products Database](#)
[ALTBIB](#)
[MEDLINEplus Tox/Env. Health](#)
[MEDLINE/PubMed](#)
[DIRLINE](#)
[NLM Gateway](#)

Support Pages

[Help](#)
[Fact Sheet](#)

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Last modified on October 1, 2003.

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ChemIDplus Record

[Tox. & Env. Health](#) [TOXNET](#) [ChemIDplus](#)

Diazepam [USAN:BAN:INN:JAN] RN: 439-14-5

For more information about this substance,
you may select from the the links below.

Basic Information

[Full
Record](#)

[Names
&
Synonyms](#)

[Formulas](#)

[Classification
Codes](#)

[Registry
Numbers](#)

[Notes](#)

Search Navigation

[Main Query
Page](#)

[Advanced
ChemIDplus
Search](#)

File Locator

[AIDSLINE](#)

[AIDS citations from MEDLINE](#)

[CANCERLIT](#)

[CANCER LITerature from Medline](#)

[CCRIS](#)

[NCI Chem Carcinogenesis Res Info System](#)

[ClinicalTrials.gov](#)

[NIH ClinicalTrials.gov](#)

[DART/ETIC](#)

[Developmental and Reproductive Toxicology](#)

[DSL](#)

[Domestic Substances List of Canada](#)

[EINECS](#)

[EU Inv of Existing Commercial Chem Sub](#)

[EMIC](#)

[Environmental Mutagen Information Center](#)

[GENETOX](#)

[EPA GENetic TOXicology](#)

[HSDB](#)

[Hazardous Substances Data Bank](#)

ChemIDplus Lite

Internet Locator

[EPA CRS](#)

[i](#) EPA Substance Registry System

[EPA Envirofacts](#)

[i](#) EPA Master Chemical Integrator

[NIAID ChemDB](#)

[i](#) NIAID Chemical Database

[NIST WebBook](#)

[i](#) NIST Chemistry WebBook

[NJ-HSFS](#)

[i](#) New Jersey Hazardous Substance Fact Sheets

Superlist Locator

[CA65](#)

[i](#) California Proposition 65 List

[DEA](#)

[i](#) DEA Controlled Substances

[IARC](#)

[i](#) International Agency for Research on Cancer

[MA](#)

[i](#) Massachusetts Right-to-know Substances

ChemIDplus Lite



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ChemIDplus Record

▶ [Tox. & Env. Health](#) ▶ [TOXNET](#) ▶ [ChemIDplus](#)

Diazepam [USAN:BAN:INN:JAN]
RN: 439-14-5

For more information about this substance,
select from the Locator/links below.

Basic Information

Full Record

Names & Synonyms

Formulas

Classification Codes

Registry Numbers

Notes



File Locator

[AIDSLINE](#)

AIDS citations from MEDLINE

[CANCERLIT](#)

NCI CANCER LITERature

[CCRIS](#)

NCI Chemical Carcinogenesis Research Information System

[ClinicalTrials.gov](#)

NIH ClinicalTrials.gov

[DART/ETIC](#)

Developmental and Reproductive Toxicology

[DSL](#)

Domestic Substances List of Canada

[EINECS](#)

EU Inventory of Existing Commercial Chemical Substances

[EMIC](#)

Environmental Mutagen Information Center

[GENETOX](#)

EPA GENetic TOXicology

[HSDB](#)

Hazardous Substances Data Bank

[MEDLINE](#)

MEDical literature onLINE

[MEDLINEplus](#)

Consumer health information

[MESH](#)

Medical Subject Headings File

[MESH HEADING](#)

Medical Subject Headings

[RTECS](#)

Registry of Toxic Effects of Chemical Substances

[TOXLINE Core](#)

NLM TOXLINE Core from MEDLINE

[TOXLINE Special](#)

NLM TOXLINE Special on TOXNET

[TSCAINV](#)

EPA Chemical Substances Inventory

HSDB ←

Download

Details

Other Files

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Help

Contents

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Expand all categories

Select

Clear

FULL RECORD

Human Health Effects

Emergency Medical Treatment

Animal Toxicity Studies

Metabolism/Pharmacokinetics

Pharmacology

Environmental Fate & Exposure

Environmental Standards & Regulations

Chemical/Physical Properties

Chemical Safety & Handling

Manufacturing/Use Information

Laboratory Methods

Special References

Synonyms and Identifiers

Administrative Information

DIAZEPAM

CASRN: 439-14-5

For other data, click on the Table of Contents

Human Health Effects:

Evidence for Carcinogenicity:

Evaluation: There is evidence suggesting a lack of carcinogenicity of diazepam to the breast and inadequate evidence for carcinogenicity at other sites in humans. There is inadequate evidence in experimental animals for the carcinogenicity of diazepam. Overall Evaluation: Diazepam is not classifiable as to its carcinogenicity in humans (Group 3). [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).p. 66 81 (1996)]**PEER REVIEWED**

Human Toxicity Excerpts:

... Studies have tended to concentrate on the suggestion that diazepam acts as a promoter in cancer, and most relate to breast cancer. No evidence of incr risk for breast cancer with diazepam use was found in a breast cancer screening study. The relative risk for 'ever' use of diazepam was 0.87 (97% confidence interval, 0.7-1.1). For use of diazepam 15 or more years earlier, the relative risk was 1.1 (0.5-2.4); for three or

ChemIDplus Lite



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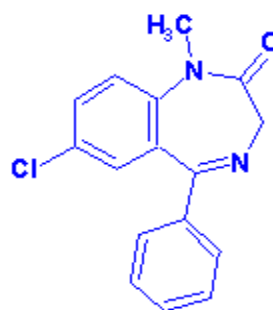
[About](#) • [Contact](#) • [Search](#)



ChemIDplus Full Record

[Tox. & Env. Health](#) [TOXNET](#) [Return to Results Page](#)

Diazepam [USAN:BAN:INN:JAN]
RN: 439-14-5



Names and Synonyms

MeSH Heading

[i](#) Diazepam

Name of Substance

[i](#) Diazepam

[i](#) Diazepam [USAN:BAN:INN:JAN]

Synonyms

[i](#) 1-Methyl-5-phenyl-7-chloro-1,3-dihydro-2H-1,4-benzodiazepin-2-one

[i](#) 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-

[i](#) 5-24-04-00300 (Beilstein Handbook Reference)

[i](#) 7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one

[i](#) 7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one (IUPAC)

[i](#) 7-Chloro-1-methyl-2-oxo-5-phenyl-3H-1,4-benzodiazepine

[i](#) 7-Chloro-1-methyl-5-3H-1,4-benzodiazepin-2(1H)-one

- WY-3467
- Winii
- Zepaxid
- Zipan
- e-Pam

Systematic Name

- 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-
- Diazepam

Superlist Name

- DEA No. 2765
- Diazepam

Formulas**Molecular Formula**

- C₁₆H₁₃ClN₂O

Classification Codes**Classification Code**

- Adjuvants, anesthesia
- Anesthetics, intravenous
- Anti-anxiety agents, benzodiazepine
- Anticonvulsants
- Antiemetics
- Drug / Therapeutic Agent
- GABA modulators
- Human Data
- Muscle relaxants, central
- Mutation data
- Reproductive Effect
- Sedative-hypnotic
- Sedatives, nonbarbiturate
- Tumor data

Superlist Classification Code

- DEA Schedule IV
- Overall Carcinogenic Evaluation: Group 3

Registry Numbers**CAS Registry Number**

- 439-14-5

Other Registry Number

- 11100-37-1
- 53320-84-6

System Generated Number

- 000439145

Notes**Note**

- A Benzodiazepine with anticonvulsant, anxiolytic, sedative, muscle relaxant, and amnesic properties and a long duration of action. Its actions are mediated by enhancement of GABA activity. It is used in the treatment of severe anxiety disorders, as a hypnotic in the short-term management of insomnia, as a sedative and premedicant, as an anticonvulsant, and in the management of alcohol withdrawal syndrome. (From Martindale, The Extra Pharmacopoeia, 30th ed, p589)

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SIS



ChemID Search Near Matches

[▶ Tox. & Env. Health](#) [▶ TOXNET](#) [▶ ChemSearch](#)
[▶ Results](#)

Your search for chemical name **"VALEUM"** did not retrieve any exact matches.

You may return to the [query page](#) and modify your search or examine any of the near matches below by clicking on it. Your search target may not be on the list.

[Valium](#)

[Valeo](#)

[Valeans](#)

[Valu-8](#)

[Valu-7](#)

[Valux](#)

[Vallene](#)

[Value 100](#)

[Valinum \[Latin\]](#)

[Vaulen](#)

[Vadern](#)

[Velium](#)

[Velmol](#)

[Vulm-411](#)

[Vulm 111](#)

[Vulm 993](#)

[VULM 993](#)

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SIS



ChemIDplus Search Results

[Tox. & Env. Health](#) [TOXNET](#) [ChemIDplus](#)

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Record
Number

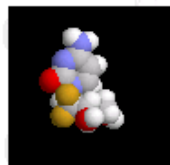
TOXNET
Home

- 1 [Nitrazepam \[USAN:BAN:INN:JAN\]](#)
146-22-5
- 2 [Diazepam \[USAN:BAN:INN:JAN\]](#)
439-14-5
- 3 [Oxazepam \[USAN:BAN:INN:JAN\]](#)
604-75-1
- 4 [Lorazepam \[USAN:BAN:INN:JAN\]](#)
846-49-1
- 5 [Temazepam \[USAN:BAN:INN\]](#)
846-50-4
- 6 [Lormetazepam \[USAN:BAN:INN:JAN\]](#)
848-75-9
- 7 [7-Aminodesmethylflunitrazepam](#)
894-76-8
- 8 [2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-3-amino-7-chloro-5-phenyl-](#)
phenyl-
894-77-9
- 9 [Demoxepam \[USAN:INN\]](#)
963-39-3
- 10 [2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-\(p-fluorophenyl\)-1-\(3-\(1-piperazinyl\)propyl\)-, hydrochloride](#)
1057-13-2

Division of Specialized Information Services, NLM
ChemIDplus Chemical Search Input Page
A [TOXNET](#) Resource

Try the new "Lite" version at
<http://chem2.sis.nlm.nih.gov/chemidplus>

- Fast searching by Name or RN
- Structures display as GIF images
- No plugin or applet required



ChemIDplus

368066 Records
206088 Structures

Powered by *Chemscape*™

<http://www.mdll.com/products/framework/chemscape/>



3D structures generated by [CORINA](#) a
product of [Molecular Networks](#)

Data Search Type:

Name/Synonym Equals

And optional [Locator Code](#) limit is

(Any)

[Structure Input Box](#)



Structure Search Type:

Substructure Search

Display Results

Display chemical structures using

Chime

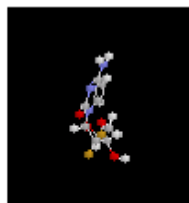
Java



ChemID*plus* Search Screen

Five drop down menus on the search screen:

- Data Search Type: Names/Synonym, Registry Number, Formula (hyphenated), Classification Code, Locator Code
- Logical Operators: Equals (the default), Starts With, Contains
- Display results: 10 (default), 25
- Locator Code (optional limit): List of files and locators, MEDLINE, TOXLINE, EPA, FDA, WHO, OSHA, CDC
- Structure Search Type: Substructure Search, Similarity Search (default 80% similarity), Exact Structure



ChemIDplus

Methyl tert-butyl ether RN: 1634-04-4

Molecular
Structure

Names and
Synonyms

Classification
Codes

Formulas

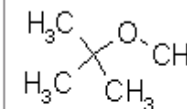
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[Enlarge Structure](#)

File Locator

- [i](#) [CANCERLIT](#)
- [i](#) [CCRIS](#)
- [i](#) [DART/ETIC](#)
- [i](#) [DSL](#)
- [i](#) [EINECS](#)
- [i](#) [EMIC](#)
- [i](#) [HSDB](#)
- [i](#) [Haz-Map](#)
- [i](#) [IRIS](#)
- [i](#) [ITER](#)
- [i](#) [MEDLINE](#)
- [i](#) [MEDLINEplus](#)
- [i](#) [MESH](#)
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- [i](#) [TOXLINE Core](#)
- [i](#) [TOXLINE Special](#)
- [i](#) [TRI2000](#)
- [i](#) [TRI2001](#)
- [i](#) [TRI95](#)
- [i](#) [TRI96](#)
- [i](#) [TRI97](#)
- [i](#) [TRI98](#)
- [i](#) [TRI99](#)
- [i](#) [TSCAINV](#)

Internet Locators

- [i](#) [ATSDR PHSs](#)
- [i](#) [ATSDR TOXFAQS](#)

[Welcome to the ChemIDplus Locator Page](#)

The [window to the left](#) displays one or more ChemIDplus Locator Codes which link to other sites that carry information about the chemical you have retrieved. [You may click on:](#)

- A hyperlinked Locator Code such as [TOXLINE](#) to retrieve data from that resource. Results will be displayed in this window.
- The information icon ([i](#)) to get a description of the source of the Locator Code and the scope of the search.

The [window on the top of the screen](#) displays buttons that you may click on to change the data displayed for this chemical or to change your search mode. Hold your mouse pointer over a button to see a more detailed description.



Locator Code Page

- Hyperlinked locators directly search resources on a substance
- Information icon (i) next to the locator gives the description of the database and scope

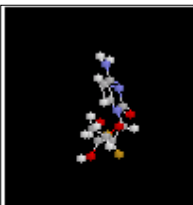


ChemIDplus

Query Results of 2

Main Query
Page

Options	ID	Structure	CAS	Molecule Name	Formula
Full Record	000081072		81-07-2	Saccharin [USAN]	C7-H5-N-O3-S
Enlarge Structure					
Use Structure For Query					
Use Structure for Similarity					
Full Record	000128449		128-44-9	Saccharin sodium anhydrous	C7-H5-N-O3-S.Na
Enlarge Structure					
Use Structure For Query					
Use Structure for Similarity					



Saccharin sodium anhydrous RN: 128-44-9

Molecular
Structure

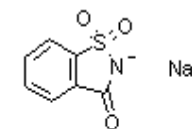
Names and
Synonyms

Classification
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[Enlarge Structure](#)

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- [i DART/ETIC](#)
- [i DSL](#)
- [i EINECS](#)
- [i EMIC](#)
- [i GENETOX](#)
- [i Household Products](#)
- [i RTECS](#)
- [i TOXLINE Special](#)
- [i TSCAINV](#)

Internet Locators

- [i EPA CRS](#)
- [i EPA Envirofacts](#)

Superlist Locator

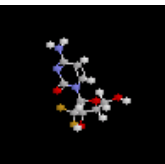
- [i HPV](#)
- [i IARC](#)
- [i INER](#)
- [i MA](#)
- [i PA](#)
- [i PAFA](#)

Welcome to the ChemIDplus Locator Page

The window to the left displays one or more ChemIDplus Locator Codes which link to other sites that carry information about the chemical you have retrieved. You may click on:

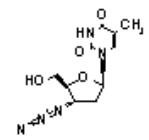
- A hyperlinked Locator Code such as [TOXLINE](#) to retrieve data from that resource. Results will be displayed in this window.
- The information icon ([i](#)) to get a description of the source of the Locator Code and the scope of the search.

The window on the top of the screen displays buttons that you may click on to change the data displayed for this chemical or to change your search mode. Hold your mouse pointer over a button to see a more detailed description.



Zidovudine [USAN:BAN:INN:JAN] RN: 30516-87-1

- [Molecular Structure](#)
- [Names and Synonyms](#)
- [Classification Codes](#)
- [Formulas](#)
- [Notes](#)
- [Registry Numbers](#)
- [Locator Codes](#)
- [Entire Record](#)
- [Main Query Page](#)



[Enlarge Structure](#)

[ChemIDplus](#)

	ID: 030516871	CAS Number: 30516-87-1
	Enlarge Structure Use Structure For Query Use Structure for Similarity	Formula: C10-H13-N5-O4

Names and Synonyms

MeSH Heading

- Zidovudine

Mixture Name

- Combivir
- Trizivir

Name of Substance

- Zidovudine
- Zidovudine [USAN:BAN:INN:JAN]

Superlist Name

- 3'-Azido-3'-deoxythymidine
- Zidovudine

Synonyms

- (component of) Combivir
- (component of) Trizivir
- 1-(3-Azido-2,3-dideoxy-beta-D-ribofuranosyl)-5-methylpyrimidine-2,4-(1H,3H)-dione
- 3'-Azido-3'-deoxythymidine
- AZT
- Azidothymidine
- BW A509U
- BW-A 509U
- CCRIS 105
- Compound S
- DRG-0004
- HSDB 6515
- NSC 602670
- Retrovir
- ZDV
- Zidovudina [Spanish]
- Zidovudine
- Zidovudinum [Latin]

Systematic Name

- Azidothymidine
- Thymidine, 3'-azido-3'-deoxy-

Classification Codes **Classification Code**

- Anti-HIV agents
- Antimetabolites
- Antimetabolites, antineoplastic
- Antiretroviral
- Antiviral
- Drug / Therapeutic Agent
- Human Data
- Mutation data
- Reproductive Effect
- Reverse transcriptase inhibitors
- Tumor data

Superlist Classification Code

- Overall Carcinogenic Evaluation: 2B

Formulas

Molecular Formula

- C10-H13-N5-O4

Locators

File Locator

- AIDS DRUGS
- AIDS LINE
- CANCER LIT
- CCRIS
- ClinicalTrials.gov
- DART/ETIC
- DSL
- EMIC
- HSDB
- MEDLINE
- MEDLINEplus
- MESH
- MESH HEADING
- RTECS
- TOXLINE Core
- TOXLINE Special

Notes

Registry Numbers

Internet Locators

- NIAID ChemDB
- NIAID HIV DRUGS
- healthfinder

Superlist Locator

- IARC
- NTPT

Note

- A dideoxynucleoside compound in which the 3'-hydroxy group on the sugar moiety has been replaced by an azido group. This modification prevents the formation of phosphodiester linkages which are needed for the completion of nucleic acid chains. The compound is a potent inhibitor of HIV replication, acting as a chain-terminator of viral DNA during reverse transcription. It improves immunologic function, partially reverses the HIV-induced neurological dysfunction, and improves certain other clinical abnormalities associated with AIDS. Its principal toxic effect is dose-dependent suppression of bone marrow, resulting in anemia and leukopenia.

CAS Registry Number

- 30516-87-1



ChemID*plus* Exercises

1. Check the file locator to see what NLM databases contain information on phenytoin. Search DART without leaving ChemID*plus*.

Type Phenytoin in search box, click Search. Click DART/ETIC in left pane under File Locator, view record in right pane.

2. Locate the record for styrene and link to the Internet Locator ATSDR TOXFAQS. Next link to the NIOSH Pocket Guide. Is styrene on the EPA Clean Air Act (CAA1)? Activate the Classification Code button and find the IARC classification on carcinogenicity, click on the "i" to see the source.

Type styrene in the search box, click Search. Scroll down the left pane and under Internet Locators click the link to ATSDR TOXFAQS. Next, scroll down and under Superlist Locator click the link to the CAA1 listing for styrene. At the top of the screen, click the button for Classification Code. Under Superlist Classification Code, click the "i" for Overall Carcinogenic Evaluation..... to view this source in the right pane.

3. Find the "valium" record in ChemID*plus* and use its structure to do substructure and similarity searches respectively. How many structures are in each category?

Type valium in the search box, click Search. Now click the Molecular Structure button at the top. Click Use Structure for Query button. Choose Similarity Search from the Structure Search Type pull-down list and click Search. Type in a percent similarity between 50 and 100, the default is 80 percent, but you may have to use a lower number if you don't retrieve any hits. For a substructure search, go back to the Structure Search page (click back button on your browser), choose Substructure Search from the Structure Search Type pull-down list, click Search

4. Identify all the HSDB records that are ozone depletors (CAA2).

Choose Locator Code from the Data Search Type pull-down list. Type HSDB in the search box. In the pull-down list that says "and optional Locator Code limit is" choose CAA2 from the pull-down list. Click Search.

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