

Chemistry lab safety information resources for academic user

Grace Baysinger (graceb@stanford.edu)

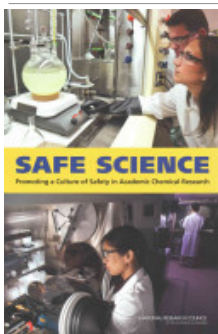
Chemistry & Chemical Engineering Librarian, Stanford University

Current Topics in Chemical Safety Information (CHAS)

Boston, MA, 18 June 2015

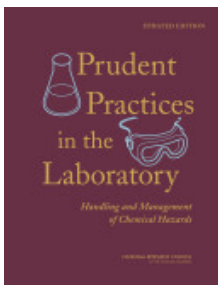


Start Here



Safe Science: Promoting a Culture of Safety In Academic Chemical Research. Washington, D.C. : National Academies Press, [2014]

http://www.nap.edu/catalog.php?record_id=18706



Prudent Practices In the Laboratory: Handling and Management of Chemical Hazards. Updated version. Washington, D.C.: National Academies Press, 2011.

http://books.nap.edu/catalog.php?record_id=12654

Outline of Topics

- Chemical Safety Data
- Reactivity, Reactions, and Protocols



Chemical Safety Data



Looking for data

- Caveats

- NA
- Provenance
- Experimental or predicted

- Searching

- Name or CAS Registry Number
- Class, Group, or Type
- Molecular Formula (Hill System Order)
 - Organic: Carbon, Hydrogen & alphabetical for all remaining elements
 - Inorganic: Alphabetical by element symbol
- Properties
 - Browse vs. search



Safety Data: International Chemical Safety Cards



Promoting safe use of chemicals in the work environment.

More than 1,700 cards are available in English. All are peer reviewed.

The National Institute of Occupational Health and Safety is a participating institution.

International Chemical Safety Cards

The cards are data sheets intended to provide essential safety and health information on chemicals in a clear and concise way. The primary aim of the cards is to promote the safe use of chemicals in the workplace. The main target users are workers and those responsible for occupational safety and health. The ICSC project is a common undertaking between the World Health Organization (WHO) and the ILO, with the cooperation of the European Commission.

Type: Database

Search for an ICSC card

ICSC number

CAS number

Chemical name or synonym

sort results by card no. chemical name

Tools

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Key resources

International Chemical Safety Card for Sodium Azide

[EN - FI - FR - HU - IT - JA - PL]

SODIUM AZIDE		ICSC: 0950 <small>Peer-Review Status: 04.07.1997 Validated</small>	
Azide Azium			
CAS #: 26628-22-8 RTECS #: VY8050000 UN #: 1687 EC #: 011-004-00-7 EINECS #: 247-852-1		Formula: NaN_3 Molecular mass: 65.02	
TYPES OF HAZARD / EXPOSURE	ACUTE HAZARDS / SYMPTOMS	PREVENTION	FIRST AID / FIRE-FIGHTING
FIRE		NO contact with acids or heavy metals.	Use dry sand, special powder.
EXPLOSION	Risk of fire and explosion on contact with acids or metals.	Do NOT expose to friction or shock.	In case of fire: keep drums, etc., cool by spraying with water.
EXPOSURE		STRICT HYGIENE!	
Inhalation	Cough. Headache. Shortness of breath. Unconsciousness. Nasal congestion. Blurred vision. Slowing of heart rate. Fall in blood pressure.	Use local exhaust or breathing protection.	Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.
Skin	MAY BE ABSORBED! Redness. Blisters.	Protective gloves.	Remove contaminated clothes. Rinse skin with plenty of water or shower.
Eyes	Redness. Pain.	Wear safety goggles or eye protection in combination with breathing protection.	First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.
Ingestion	Abdominal pain. Nausea. Sweating. Further see Inhalation.	Do not eat, drink, or smoke during work.	Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Rest. Refer for medical attention .

International Chemical Safety Card for Sodium Azide cont.

SPILLAGE DISPOSAL	PACKAGING & LABELLING
<p>Evacuate danger areal Consult an expert! Sweep spilled substance into covered plastic containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Personal protection: complete protective clothing including self-contained breathing apparatus.</p>	<p>Do not transport with food and feedstuffs. EC Classification Symbol: T+, N; R: 28-32-50/53; S: (1/2)-28-45-60-61 UN Classification UN Hazard Class: 6.1; UN Pack Group: II GHS Classification</p>
EMERGENCY RESPONSE	SAFE STORAGE
<p>Transport Emergency Card: TEC (R)-61G12B.</p>	<p>Fireproof. Separated from acids, food and feedstuffs, metals, lead and lead compounds.</p>
IMPORTANT DATA	
<p>Physical State; Appearance ODOURLESS COLOURLESS HEXAGONAL CRYSTALS.</p> <p>Physical dangers</p> <p>Chemical dangers May explode on heating above melting point, especially on rapid heating. This generates fire and explosion hazard. The solution in water is a weak base. Reacts with copper, lead, silver, mercury and carbon disulfide. This produces particularly shock-sensitive compounds. Reacts with acids. This produces toxic and explosive hydrogen azide.</p> <p>Occupational exposure limits TLV: 0.29mg/m³ (ceiling value); A4 (not classifiable as a human carcinogen); (ACGIH 2005).</p>	<p>Routes of exposure The substance can be absorbed into the body by inhalation, through the skin and by ingestion.</p> <p>Inhalation risk Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly.</p> <p>Effects of short-term exposure The substance is irritating to the eyes, skin and respiratory tract. Exposure slightly above the OEL could cause effects on the nervous system.</p> <p>Effects of long-term or repeated exposure</p>
PHYSICAL PROPERTIES	ENVIRONMENTAL DATA
<p>Decomposes at 275°C Relative density (water = 1): 1.8475 Solubility in water, g/100ml at 17°C: 41.7 (good)</p>	



PubChem

NIH > U.S. National Library of Medicine > National Center for Biotechnology Information

PubChem | OPEN
CHEMISTRY
DATABASE

SEARCH 1.0 β ETA [Current System](#)



PubChem – ID plus ToC for Sodium Azide

NIH U.S. National Library of Medicine National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE Search

Compound Summary for CID 33557

Sodium Azide

Vendors Pharmacology Literature Patents Bioactivities

PubChem CID:	33557
Chemical Names:	sodium azide; Azide, sodium; 26628-22-8; SMITE; azidosodium; Natriumazid; More...
Molecular Formula:	N_3Na
Molecular Weight:	65.009869 g/mol
InChI Key:	PXIPVTKHYLBLMZ-UHFFFAOYSA-N
UNII:	968JJ8C9DV
Modify Date:	2015-04-19
Create Date:	2005-08-01

A cytochrome oxidase inhibitor which is a nitridizing agent and an inhibitor of terminal oxidation. (From Merck Index, 12th ed)

Contents

- 1 2D Structure
- 2 3D Status
- 3 Identification
- 4 Chemical and Physical Properties
- 5 Related Records
- 6 Chemical Vendors
- 7 Pharmacology and Biochemistry
- 8 Use and Manufacturing
- 9 Safety and Hazards
- 10 Toxicity
- 11 Literature
- 12 Patents
- 13 Biological Test Results
- 14 Classification
- 15 Information Sources

PubChem – excerpt from entry on Sodium Azide

9.1.5 Inhalation Hazard

Cough. Headache. Shortness of breath. Unconsciousness. Nasal congestion. Blurred vision. Slowing of heart rate. Fall in blood pressure. *from ILO-ICSC [5]*

9.1.6 Eye Hazard

Redness. Pain. *from ILO-ICSC [5]*

9.1.7 Ingestion Hazard

Abdominal pain. Nausea. Sweating. Further see Inhalation. *from ILO-ICSC [5]*

9.1.8 Fire Potential

NOT CONSIDERED FLAMMABLE UNLESS HEATED ABOVE 300 DEG C.

Weed Science Society of America. Herbicide Handbook. 5th ed. Champaign, Illinois: Weed Science Society of America, 1983., p. 439

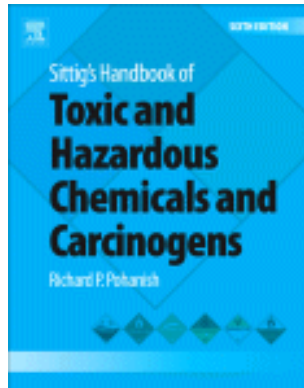
from HSDB [1]

9.2 Safety and Hazard Properties

9.2.1 Flammability

Combustible Solid (if heated above 572°F). *from NIOSH-PocketGuide [7]*

Sittig's Handbook of Toxic and Hazardous Chemicals and Carcinogens



One of the most reliable, easy-to-use and essential reference works on hazardous materials.

Providing a vast array of critical information on the 2,100 most heavily used, transported, and regulated chemical substances of both occupational and environmental concern.

Arranged alphabetically by name of substance.

Available in print and online at Stanford.

Sittig's: Excerpts from entry for Sodium Azide

Sodium azide

S:0390

Molecular Formula: N_3Na

Common Formula: NaN_3

Synonyms: AI3-50436; Axiom; Azida sodico (Spanish); Azide; Azium; Azoture de sodium (French); Dazoe; Hydrazoic acid, Sodium salt; Kazoe; Natriumazid (German); NCI-C06462; Smite; Sodium salt of hydrazoic acid

CAS Registry Number: 26628-22-8; (*alt.*) 12136-89-9

Description: Sodium azide is a colorless to white, odorless, crystalline solid. Combustible solid above 300°C. Molecular weight = 65.02; Specific gravity ($\text{H}_2\text{O}:1$) = 1.85 at 25°C; Boiling point = (decomposes); Freezing/Melting point = (the solid crystals decompose with the evolution of nitrogen gas, leaving a residue of sodium oxide) 275°C. Hazard Identification (based on NFPA-704 M Rating System): Health 4, Flammability 0, Reactivity 2. Soluble in water; reaction; solubility = 42% at 17°C.

Incompatibilities: Reacts explosively and/or forms explosive and/or shock-sensitive compounds with acids and many metals. Contact with water forms hydrazoic acid. Combustible solid (if heated above 300°C). May explode when heated above its melting point, especially if heating is rapid. Reacts with acids, producing toxic, shock-sensitive, and explosive hydrogen azide. It forms explosive compounds with phosgene, brass, zinc, trifluoroacryloyl fluoride, and nitrogen-diluted bromine vapor. Reacts with benzoyl chloride and potassium hydroxide, bromine, carbon disulfide, copper, lead, nitric acid, barium carbonate, sulfuric acid, chromium(II) hypochlorite, dimethyl sulfate, dibromomalononitrile, silver, mercury. Over a period of time, sodium azide may react with copper, lead, brass, or solder in plumbing systems to form an accumulation of the *highly explosive* and shock-sensitive compounds of lead azide and copper azide.

Sittig's: Excerpts from entry for Sodium Azide cont.

Personal Protective Methods: Wear protective gloves and clothing to prevent any reasonable probability of skin contact. Safety equipment suppliers/manufacturers can provide recommendations on the most protective glove/clothing material for your operation. All protective clothing (suits, gloves, footwear, headgear) should be clean, available each day, and put on before work. Contact lenses should not be worn when working with this chemical. Wear dust-proof goggles and face shield when working with powders or dust, unless full face-piece respiratory protection is worn. Where sodium azide may be present in solution, wear splash-proof chemical goggles and face shield, unless full face-piece respiratory protection is worn. Employees should wash immediately with soap when skin is wet or contaminated. Provide emergency showers and eyewash.

Respirator Selection: Where there is potential for exposures over 0.1 ppm as a dust, fume, or mist, use a NIOSH/MSHA- or European Standard EN149-approved full face-piece respirator with a high-efficiency particulate filter. Greater protection is provided by a powered air-purifying respirator. *Where there is potential for high exposures*, or for exposures to hydrazoic acid vapor, use a NIOSH/MSHA- or European Standard EN149-approved supplied-air respirator with a full face-piece operated in the positive-pressure mode, or with a full face-piece, hood, or helmet in the continuous-flow mode; or use a NIOSH/MSHA- or European Standard EN149-approved self-contained breathing apparatus with a full face-piece operated in pressure-demand or other positive-pressure mode.

WebWISER

NIH U.S. National Library of Medicine
Specialized Information Services


WISER 

**Wireless Information System
for Emergency Responders**

WebWISER Home | Substance List | Help Identify | Tools | Help

Current Profile  1st Responder

[WebWISER PDA and Screen Reader Access](#)

Select your profile to customize WISER's content to better suit your role in an emergency. 

Welcome to WebWISER

WISER is a system designed to assist emergency responders in hazardous material incidents. WISER provides a wide range of information on hazardous substances, including substance identification support, physical characteristics, human health information, and containment and suppression advice. To get started, configure your profile and select an item below.

Known Substances

Search for a substance within WISER's database of known substances.

Help Identify Chemical

Identify an unknown chemical based on its physical properties, symptoms of exposure, the environment, and other criteria.

Tools

Explore general tools and reference material.



Other Chemical Emergency Resources at NLM

- Chemical Hazards Emergency Medical Management (CHEMM)
- Radiation Emergency Medical Management (REMM)
- TOXNET
- MedlinePlus offers trusted links to general health topics
 - Fire Safety
 - Disaster Preparation and Recovery
 - Poisoning
 - and more...
- Household Products Database
- Tox Town
- Other Environmental Health Topics

WebWISER is best viewed with the following browsers (indicated version or higher): Internet Explorer 7, Firefox 24, Safari 5, or Google Chrome 30.

CCOHS Web Information Service



CCOHS Home | Web Information Service | Search Results

sodium azide Results per page: 20

Searched Web Information Service for **sodium azide**:

[Help - Search Results](#)

Summary

Marked Records

MSDS

CHEMINFO

CHEMpendium

RTECS

OSH References

Legislation

Additional Resources

#	Web Collections	Description
48	MSDS	Material Safety Data Sheets [About...]
19	CHEMINFO	Comprehensive health and safety information on pure chemicals [About...]
187	CHEMpendium	Chemical databases [About...]
1	RTECS	Registry of Toxic Effects of Chemical Substances [About...]
109	OSH References	Bibliographic references [About...]
19	Legislation	Canadian enviroOSH legislation plus Standards [About...]

#	Additional Resources	Description
8	CHEMINDEX	CAS Registry Numbers [About...]
49	OSH Answers	Questions and answers about occupational health and safety topics [About...]
206	INCHEM	Internationally peer reviewed information from intergovernmental organizations [About...]
3	ILO Encyclopaedia	ILO Encyclopaedia of Occupational Health and Safety [About...]

Knovel

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Knovel® Search sodium azide Data Search

New Interactive Equations Available Now! Find equations paired with worked examples and use built-in software to perform calculations Try It Now

Home Search for 'sodium azide' Search within these results


Save Search All Content My Subscription Relevancy Date Page 1 of 28

TECHNICAL REFERENCES

- All Technical References
- Text Sections (238)
- Interactive Tables (20)
- Interactive Graphs (17)
- Conference Proceedings (2)

DICTIONARY/ENCYCLOPEDIA + Save to My Knovel


sodium azide

 from Dictionary of Science (6th Edition) (2010)
See more results from this title | Search within this title »

TEXT SECTIONS + Save to My Knovel

Sodium Azide

...include oxides of nitrogen and **sodium** oxide. Reactivity and Incompatibility **Sodium azide** should not be allowed to come into contact with heavy metals or their salts, because... more »

 from Prudent Practices in the Laboratory - Handling and Disposal of Chemicals (1995)
See more results from this title | Search within this title »

eChemPortal



Print

English ▾

The Global Portal to Information on Chemical Substances



eChemPortal

eChemPortal ▾

› Home

› Substance Search

› Property Search

› What's new?

› General Information

› Participating Databases

› Roles & Responsibilities

› Extension of the Portal

› Linking to eChemPortal

› Schedules of Assessments

› Structure Search

› GHS Classifications

› Other useful information

› FAQ

› Help

› Contact us

› Disclaimer

Chemical Substance Search

Twenty-nine data sources participate under Chemical Substance Search.

Four databases participate under Chemical Property Data Search.

Chemical Property Data Search

The [list of data sources participating](#) in eChemPortal is continuously expanding.

*Help us to help you.
Answer the [User Survey](#)*

eChemPortal provides free public access to information on properties of chemicals:

- Physical Chemical Properties
- Environmental Fate and Behaviour
- Ecotoxicity
- Toxicity

eChemPortal allows simultaneous searching of reports and datasets by chemical name and number and by chemical property. Direct links to collections




Latest news

Closure of ESIS and OECD SIDS temporarily down

17 November 2014

The Joint Substance Data Pool of the German Federal Government and the German Federal States is now linked to eChemPortal

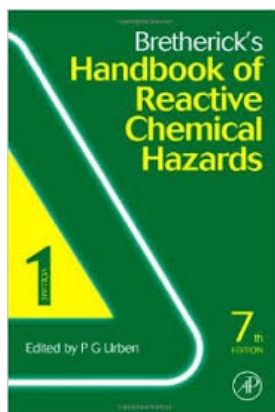
More Resources

- **Canadian Centre for Occupational Health and Safety. Web Information Service** - metasearch for chemical hazard information from many sources. 
- **Knovel** – site contains 2,000+ handbooks. Browse or search the Safety and Industrial Hygiene section. Provided by Knovel. 
- **Encyclopedia of Reagents for Organic Synthesis** – includes safety information. Provided by Wiley. 
- **Hazardous Substances Data Bank** - HSDB has comprehensive, peer-reviewed toxicology data for about 5,000 potentially hazardous chemicals. Provided by NLM.
- **eChemPortal** - provides free public access to information on properties of chemicals: Physical Chemical Properties, Ecotoxicity, Environmental Fate and Behavior, and Toxicity. Provided by the OECD.

Reactivity, Reactions, and Protocols



Reactivity Information – Bretherick's Volume 1



Bretherick's Handbook of Reactive Chemical Hazards (print + online as PDF)

Two volume set. V.1=Specific Chemicals. V. 2=Class, Group, & Topic.

Find stability of single compound:

- Elements and substances are arranged by molecular formula in volume 1.
- Use Volume 1, Appendix 4 (Index of Chemical Names & Synonyms). Browse by name and find entry number.
- In the online version, search entry number followed by name (example: 4753. Sodium Azide). Open PDF for chapter in search results and then use Cntrl-F to locate entry.

Find data on possible violent interaction between two or more compounds.


- Determine which compound is more reactive (using above method).
- Browse sub-entries for that compound (e.g. Sodium Azide, Barium Carbonate).

For more information about specific chemicals, see:

- Appendix 2: Fire-related data
- Appendix 5: CAS Registry Number Index

Search Results in the Online Version of Bretherick's

ScienceDirect Journals Books

4753. Sodium Azide Author name --This Journal/Book-- Volume Issue Page  Advanced search

Search results: 6 results found. [See image results](#)

Did you mean: ALL(4753. Sodium *oxide*)



Refine filters



Year

- 2007 (6)

Publication title

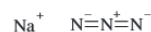
- Bretherick's Handbook of Reactive Chemical Haza... (6)

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- N**
Bretherick's Handbook of Reactive Chemical Hazards (Seventh Edition), Volume 1, 2007, Pages 1863-1925
[First page PDF](#) |  [PDF \(252 K\)](#)
- M**
Bretherick's Handbook of Reactive Chemical Hazards (Seventh Edition), Volume 2, 2007, Pages 206-251
[First page PDF](#) |  [PDF \(164 K\)](#)

Bretherick's entry on Sodium Azide (in Vol. 1)

4753. Sodium azide [26628-22-8]



HCS 1980, 827

1. Mellor, 1940, Vol. 8, 345
2. Lambert, B., *School Sci. Rev.*, 1927, **8**(31), 218
3. Anon., *Jahresber.*, 1981, 77—79
4. Anon., *Safety*, 1982, (3), 2
5. Grewer, T. *et al.*, *Exothermic Decomposition*, Technical Report 01VD 159/0329 for Federal German Ministry for Res. Technol., Bonn. 1986
6. www.chemsafety.gov/circ. US Chem. Safety & Haz. Investigation Board, CSB 2001-5086
7. Hagenbuch, J-P. *Chimia*, 2003, **57**(12), 773

Insensitive to impact, it decomposes, sometimes explosively, above its m.p. [1], particularly if heated rapidly [2]. Although used in aqueous solutions as a preservative in pharmaceutical preparations, application of freeze-drying techniques to such solutions has led to problems arising from volatilisation of traces of hydrazoic acid from non-neutral solutions, condensation in metal lines, traps or filters, and formation of

heavy metal azides in contact with lead, copper or zinc components in the drying plant [3,4]. An explosion is reported when cutting into a pipe previously used to transport the powdered azide [air may have been involved as an oxidant – Ed.] [6]. A study of risks inherent in industrial use of sodium azide at hundred kg scale is reported. For reagent use, keeping the mix buffered to alkalinity is important [7]

Energy of exothermic decomposition in range 230—260°C was measured as 0.76 kJ/g by DSC, and $T_{\text{ait}24}$ was determined as 253°C by adiabatic Dewar tests, with an apparent energy of activation of 145 kJ/mol [5].

See Heavy metals, below

Acids

See Hydrogen azide

Ammonium chloride, Trichloroacetonitrile

See 5-Trichloromethyltetrazole

Barium carbonate

Henneburg, G. O. *et al.*, *Can. J. Res.*, 1950, **28B**, 345

Interaction to form cyanide ion requires careful control of temperature at 630°C to prevent explosions.

Bromine

See Bromine: Metal azides



Reactivity - Bretherick's Volume 2

Volume 2: Class, Group and Topic 

- Appendix 3: Alphabetical Index
- Appendix 4: Classified by Type Index
 - Chemical Classes
 - Inorganic chemical groups
 - Organometallic chemical groups
 -  ◦ Organic chemical groups
 - Hybrid chemical groups
 - Hazard Assessment and prediction topics
 - Miscellaneous topics
 - Performance materials topics
 - Phenomenon topics
 - Specific reaction hazards
 - Substances (not simple chemical entities, often of natural origin)
 - Technique topics
 - Unit operation or process topics

METAL AZIDES

MN₃

1. Mellor, 1940, Vol. 8, Suppl. 2, 16—54
2. *Energetic Materials*, Fair, H. D. and Walker, R. F. (Eds.), Vols. 1 and 2, New York, Plenum, 1977

This large and well documented group of explosive compounds contains some which are widely used industrially [1]. The text gives a thorough treatment of all aspects of the physics and chemistry (Vol. 1) and of the applications (Vol. 2) of this important group of energetic compounds [2] and individually indexed compounds are:

- Aluminium azide, 0082
- * Azidogermane, 4410
- Barium azide, 0214
- * Bis(2-aminoethyl)aminocobalt(III) azide, 1769
- * Bis(cyclopentadienyl)tungsten diazide oxide, 3279



Organic Chemical Groups

ACETYLENIC COMPOUNDS, 2
ACETYLENIC PEROXIDES, 5
ACRYLIC MONOMERS, 6
O-ACYLHYDROXAMIC ACIDS, 9
ACYL HYPOHALITES, 10
ACYL NITRATES, 10
ACYL NITRITES, 10
ALDEHYDES, 12

CAMEO Chemicals

CAMEO *Chemicals*


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New Search


MyChemicals
chemicals: 0
View MyChemicals
Predict Reactivity

Mobile Site

Database of Hazardous Materials

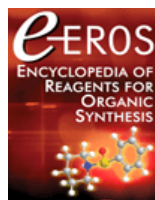
 [Search](#)
Find response information for thousands of hazardous materials, including fire and explosion hazards, health hazards, firefighting techniques, cleanup procedures, protective clothing, and chemical properties.

 [MyChemicals](#)
Build a list of chemicals. For example, substances involved in an incident response (such as a train derailment) or chemicals stored in your community.

 [Reactivity](#)
See what hazards might occur if chemicals in your MyChemicals collection are mixed together.



e-EROS: Encyclopedia of Reagents for Organic Synthesis



- *e-EROS* has in-depth information on reagents and catalysts for all chemists planning or working on organic syntheses.
- *e-EROS* gives detailed information on more than 4,500 reagents and catalysts, and every year more than 200 new or updated articles are added in order to keep the Database up-to-date.
- Search by Reagent Name or Chemical Structure. Entries include safety information.

Sodium Azide¹



[26628-22-8] N₃Na (MW 65.02)
InChI = 1/N3.Na/c1-3-2;/q-1;+1
InChIKey = PXIPVTKHYL.BLMZ-UHFFFAOYAH

(nucleophilic azide source for organoazide preparation;² precursor to reagents such as hydrazoic acid,³ halogen azides,⁴ trimethylsilyl azide,⁵ tosyl azide,⁶ and diphenyl phosphorazidate⁷)

Physical Data: dec ca. 300 °C; *d* 1.850 g cm⁻³.

Solubility: sol water (39 g/100 g at 0 °C, 55 g/100 g 100 °C); slightly sol alcohol; insol ether.

Form Supplied in: white solid; widely available.

➔ *Handling, Storage, and Precautions:* while relatively insensitive to impact, the solid can decompose explosively above its melting point. It forms highly explosive azides with metals such as Cu, Pb, Hg, Ag, Au, their alloys and compounds, and reacts with acids to form hydrazoic acid (HN₃) which is a toxic, spontaneously explosive gas. Explosive *gem*-diazides can be formed in CH₂Cl₂ or other chlorinated solvents and shock or heat sensitive metal azidothioformates in CS₂. All work with NaN₃ and other azides should be conducted on a very small scale behind a shield, in a fume hood. Excess NaN₃ on flasks, paper, etc. can be destroyed in a fume hood by soaking with acidified *Sodium Nitrite* or by oxidation with *Cerium(IV) Ammonium Nitrate*.⁸

e-EROS – Structure Search page

Wiley Online Library SUL [Log in / Register](#)

Home > Organic Chemistry > Methods - Synthesis & Techniques > e-EROS Encyclopedia of Reagents for Organic Synthesis

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e-EROS Encyclopedia of Reagents for Organic Synthesis

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Online ISBN: 9780470842898
DOI: 10.1002/047084289X

Name/Identifier Draw/Upload

Structure Properties*Molecular weight, molecular formula*

Reaction Properties*Reaction Keyword, Catalyst, Solvent, Temperature, Yield*

Literature Filters*FullText, Article Title, Author, Publication Date*

SEARCH

All content

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Search in this Database >
[Chemistry Structure Search >](#)



e-EROS – Search Results using Name in Structure Search form

Home > Advanced Search

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Book Home

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Reagent Name
Structure Search

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Editors & Contributors

SPECIAL FEATURES

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EROS Best Reagent Award
Most Popular Reagents

e-EROS Encyclopedia of Reagents for Organic Synthesis

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Online ISBN: 9780470842898

DOI: 10.1002/047084289X

Current Search

You searched for: **sodium azide**

EDIT SEARCH

NEW SEARCH

143 literature results for name/identifier search

Best Match

Go

VIEW 1 - 20 | 21 - 40 | 41 - 60 | 61 - 80 | next >

There are 143 results

Sodium Azide

Encyclopedia of Reagents for Organic Synthesis

Kenneth Turnbull, B. Narsalah, J. S. Yadav, T. Yakaiah and B. P. V. Lingaiah

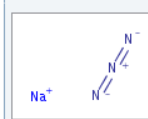
Published Online: 14 MAR 2008, DOI: 10.1002/047084289X.rs045.pub2

Abstract | Full Article (HTML) | Enhanced Article (HTML) | PDF(139K)
References



Matching compounds (1)

Matching reactions (58)



SEARCH

All content

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Chemistry Structure Search >

Wiley Chemistry Structure Search Results

http://
onlinelibrary.wiley.com/
chemistry/search

Home > Advanced Search

Chemistry Search | Search Tips
Search selected Online Library chemistry journals by chemical compounds and reactions.

Current Search

You searched for: **sodium azide** EDIT SEARCH NEW SEARCH

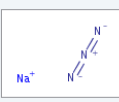
351 literature results for name/identifier search Best Match Go

VIEW 1 - 20 | 21 - 40 | 41 - 60 | 61 - 80 | next >

There are 351 results

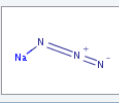
Electrophilic Amination of Carbanions, Enolates, and Their Surrogates
Organic Reactions
Engelbert Ciganek
Published Online : 16 MAR 2009, DOI: [10.1002/0471264180.or072.01](https://doi.org/10.1002/0471264180.or072.01)
Abstract | **Full Article (HTML)** | **Enhanced Article (HTML)** | **PDF(923K)** | **References**

Matching compounds (1) **Matching reactions (20)**



Hydrazoic Acid and Azides
Ullmann's Encyclopedia of Industrial Chemistry
Horst H. Jobelius and Hans-Dieter Scharff
Published Online : 15 JUN 2000, DOI: [10.1002/14356007.a13_193](https://doi.org/10.1002/14356007.a13_193)
Abstract | **Full Article (HTML)** | **Enhanced Article (HTML)** | **PDF(91K)** | **References**

Matching compounds (1)



Sodium Azide
Encyclopedia of Reagents for Organic Synthesis

REACTIONS

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[Refine](#)

Group by: Transformation Sort by: Frequency

0 of 2040 Reactions Selected

Analyze by:

Reagent

 Et₃N 1263

AcOH 1167

HCl 1147

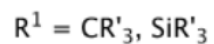
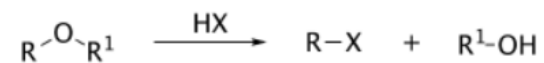
 (Me₃Si)₂NH •Li 1143

 NaHCO₃ 1102

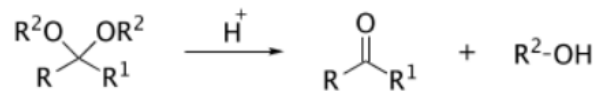
 H₂ 884

t-BuOK 813

1. Formation of Alkyl Halides/ Alcohols from Ethers / Silyl Ethers 60 Reactions



2. Hydrolysis of Acetals/ Orthoesters/ Enol Ethers and Similar Compounds 43 Reactions



SF

Substance Identifier "taxol " > substances (1) > **get reactions (2040)** > keep analysis "Experimental Procedure" (683)

REACTIONS

Get References Tools

Analyze **Refine**

Analyze by: Experimental Procedure

Experimental Procedures Not Available 1357

Experimental Procedures Available 683

Group by: Transformation Sort by: Frequency

0 of 2040 Reactions Selected

1. Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers
60 Reactions

$$\text{R-O-R}^1 \xrightarrow{\text{HX}} \text{R-X} + \text{R}^1\text{-OH}$$

$\text{R}^1 = \text{CR}'_3, \text{SiR}'_3$

2. Hydrolysis of Acetals/ Orthoesters/ Enol Ethers and Similar Compounds
43 Reactions

$$\begin{array}{c} \text{R}^2\text{O} \\ | \\ \text{R}-\text{C}-\text{OR}^2 \\ | \\ \text{R}^1 \end{array} \xrightarrow{\text{H}^+} \begin{array}{c} \text{O} \\ || \\ \text{R}-\text{C}-\text{R}^1 \end{array} + \text{R}^2\text{-OH}$$
$$\begin{array}{c} \text{R} \\ | \\ \text{R}-\text{C}=\text{C}-\text{OR}^1 \\ | \\ \text{R} \end{array} \xrightarrow{\text{H}^+} \begin{array}{c} \text{R} \\ | \\ \text{R}-\text{C}-\text{C}-\text{R} \\ | \quad || \\ \text{R} \quad \text{O} \end{array} + \text{R}^1\text{-OH}$$

SF

Substance Identifier "taxol" > substances (1) > get reactions (2040) > keep analysis "Experimental Procedure" (683) > keep analysis "Journal Name" (14)

REACTIONS

Get
References

Tools

Analyze Refine

Group by: Document Sort by: Accession Number

Analyze by:

Journal Name

Journal of the
American Chemical
Society 14

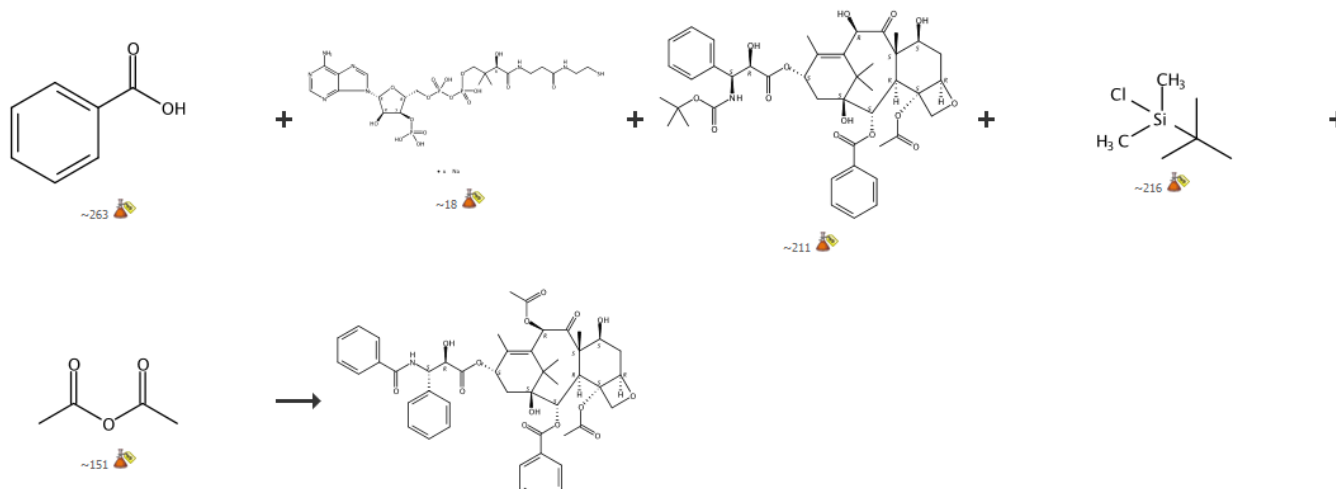
Show More

0 of 14 Reactions Selected

1. An N-Aroyltransferase of the BAHD Superfamily Has Broad Aroyl CoA Specificity in Vitro with Analogues of N-Dearoylpaclitaxel

[Quick View](#) [Other Sources](#)

12 Reactions

6 Steps (Converging) *Hover over any structure for more options.*

SF

▼ Overview

Steps/Stages

- 1.1 R:Et₃N, S:THF, S:CH₂Cl₂, 10 min, 23°C
- 1.2 R:ClCO₂Et, 1 h, 23°C
- 1.3 R:NaHCO₃, S:H₂O, S:*t*-BuOH, 0.5 h, 23°C
- 1.4 R:HCl, S:H₂O, pH 3-5
- 1.1 R:1H-Imidazole, S:DMF, 18 h, 23°C
- 2.1 R:CeCl₃•7H₂O, S:THF, rt; 1 h, rt
- 3.1 R:C₅H₅N, R:HF, S:THF, S:C₅H₅N, 0°C; 0°C → rt; 10 h, rt
- 4.1 R:HCO₂H, S:H₂O, S:MeCN, 0°C; 0°C → rt; 4 h, rt
- 4.2 R:NaHCO₃, S:H₂O, S:CHCl₃
- 5.1 R:Glycerol, C:476683-00-8, S:H₂O, pH 8
- 5.2 R:HCl, S:H₂O, 2.5 h, rt

Notes

regioselective, regioselective, incremental addition of pyridine and HF, enzymic, biotransformation, sodium phosphate buffered solution used, recombinant N-debenzoyl-2'-deoxytaxel:N-benzoyltransferase from *Taxus* plants overexpressed in *Escherichia coli* used, kinetic study, Reactants: 5, Reagents: 10, Catalysts: 1, Solvents: 8, Steps: 6, Stages: 11, Most stages in any one step: 4

References

[An N-Aroyltransferase of the BAHD Superfamily Has Broad Aroyl CoA Specificity in Vitro with Analogues of N-Deaoylpaclitaxel](#)

[Quick View](#) [Other Sources](#)

By Nevarez, Danielle M. et al

From Journal of the American Chemical Society, 131(16), 5994-6002; 2009

▼ Experimental Procedure



Sequence 1

Step 1

Synthesis of CoA Thioesters. Several aroyl CoA donors (heteroaroyls and variously substituted benzoyls) were synthesized *via* a previously described method that proceeds through a mixed ethyl carbonate anhydride.²⁹ Briefly, triethylamine (3.0 μL, 30 μmol) was added to a solution of the corresponding carboxylic acid (27 μmol) in 5:2 CH₂Cl₂/THF (v/v, 1.4 mL) under N₂ gas. The mixture was stirred for 10 min at 23 °C, ethyl chloroformate (2.9 μL, 30 μmol) was added in one portion, and the reaction was stirred for 1 h at 23 °C. The solvents were evaporated under reduced pressure, and the residue was dissolved in 0.5 mL of *tert*-butyl alcohol. Coenzyme A as the sodium salt (23 mg, 30 μmol dissolved in 0.5 mL of 0.4 M NaHCO₃) was added to the solution, and the mixture was stirred for 0.5 h at 23 °C, then quenched with dropwise addition of 1 M HCl, and adjusted to pH 3-5. The solvents were evaporated under vacuum, and the residue was dissolved in water (5 mL, pH 5) and loaded onto a C18 silica gel column (10% capped with TMS) that was washed with 100% MeOH (50 mL) and preequilibrated with distilled water (100 mL, pH 5). The sample was washed with water (100 mL, pH 5) and then eluted with 15% MeOH in water (50 mL, pH 5). The fractions containing aroyl CoA, as determined by TLC, were combined, and the solvent was evaporated to yield product (95-99% yield at 95-99% purity, assessed by ¹H NMR) (see Supporting Information).

Synthesis of benzoyl CoA. The product was isolated in >99% yield (99% pure by ¹H NMR). ESI-MS (negative ion mode), *m/z*: 870.1 (M-H), 434.5 (M-2H)², 289.3 (M-3H)³. ¹H NMR (300 MHz, D₂O) δ: 0.58 (s, H-10'), 0.71 (s, H-11'), 2.27 (t, *J* = 7.2 Hz, H-4'), 2.98 (t, *J* = 7.2 Hz, H-1'), 3.27 (m,


Reaxys – Searched Taxol as a product, limited results to JACS and sorted by Year



The screenshot displays the Reaxys search results interface. At the top, a navigation bar includes links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this, a workflow diagram shows the search process: starting with a 'Query' (represented by a magnifying glass over chemical structures), leading to '330 reactions', then '330 reactions sorted by Publication Year', and finally '94 reactions filtered by Journal Title'. A 'Create Alert' button is visible under the query step.

Below the workflow, there is an 'Open Analysis View' button with a bar chart icon. The main results section shows '94 reactions out of 100 substances and 6 citations'. On the left, a 'Filter by:' section includes options for Substructure, Yield, and Record Type. The main results area has tabs for 'Reactions', 'Substances (Grid)', 'Substances (Report)', and 'Citations'. The 'Reactions' tab is active, showing a toolbar with icons for Limit to, Exclude, Export, Print, Zoom in, Zoom out, and Hide. The 'Sort by' dropdown is set to 'Publication Year'. Below the toolbar, there are sections for 'Yield', 'Conditions', and 'References'.

Reaxys Search Results

90%	With hydrogenchloride in methanol; water T=-5 - 30°C; 27 h; Hide Experimental Procedure	Kung, Liang-Rern; Chang, Shih-Sheng; Fang, Tung-Shen; Lin, Shu-Fen; Chang, Cheng-Chang; Chen, Chia-Hui; Hung, Yi-Ting; Cheng, Ming-Ching Patent: US2012/149925 A1, 2012 ; Location in patent: Page/Page column 15 ; Title/Abstract Full Text Show Details
	22: The crude T3 of EXAMPLE 14 in 22.5 mL MeOH was added 0.09 mL 32percent HCl _(aq) at -55° C. and then the reaction mixture was stirred for 3 hours. As the reaction temperature was raised to 2030° C., the reaction mixture was stirred for 24 hours until the deprotection was completed. The reaction mixture was dried by rotavapor and then diluted with 40 mL CH ₂ Cl ₂ . After washed with 40 mL saturated sodium bicarbonate, the organic layer was dried by rotavapor to obtain the crude. The crude in 10 mL CH ₂ Cl ₂ was slowly added 20 mL n-heptane to let paclitaxel precipitate. After filtration and dried the solid, 7.0 g paclitaxel (yield 90percent, LC purity 95percent) was obtained. ¹ H NMR (400 MHz, CDCl ₃) δ 8.14 (d, J=7.2 Hz, 2H), 7.75 (d, J=7.2 Hz, 2H), 7.63-7.56 (m, 1H), 7.53-7.47 (m, 5H), 7.43-7.34 (m, 5H), 7.00 (d, J=8.8 Hz, 1H), 6.27 (s, 1H), 6.25 (dd, J=8.0 and 9.2 Hz, 1H), 5.80 (dd, J=2.8 and 9.2 Hz, 1H), 5.68 (d, J=7.2 Hz, 1H), 4.95 (dd, J=1.6 and 9.6 Hz, 1H), 4.80 (dd, J=2.8 and 5.2 Hz, 1H), 4.42-4.37 (m, 1H), 4.31 (d, J=8.4 Hz, 1H), 4.20 (d, J=8.4 Hz, 1H), 3.80 (d, J=7.2 Hz, 1H), 3.58 (d, J=5.2 Hz, 1H), 2.58-2.50 (m, 1H), 2.47 (d, J=4.0 Hz, 1H), 2.38 (s, 3H), 2.36-2.27 (m, 2H), 2.23 (s, 3H), 1.91-1.84 (m, 1H), 1.79 (s, 3H), 1.68 (s, 3H), 1.24 (s, 3H), 1.14 (s, 3H); ¹³ C NMR (100 MHz, CDCl ₃) δ 203.6, 172.7, 171.3, 170.3, 167.07 167.02, 142.0, 137.9, 133.7, 133.6, 133.1, 132.0, 130.2, 129.1, 129.0, 128.7, 128.4, 127.0, 84.4, 81.1, 79.0, 76.5, 75.5, 74.9, 73.2, 72.3, 72.2, 58.6, 55.0, 45.6 43.1 35.68, 35.62, 26.8, 22.6, 21.8, 20.8, 14.8, 9.5. Hide Details	
80%	With pyridine hydrogenfluoride in tetrahydrofuran T=25°C; 1.25 h;	Nicolaou; Nantermet; Ueno; Guy Journal of the Chemical Society - Series Chemical Communications, 1994 , # 3 p. 295 - 296 Title/Abstract Full Text View citing articles Show Details Nicolaou; Nantermet; Ueno; Guy; Couladouros; Sorensen Journal of the American Chemical Society, 1995 , vol. 117, # 2 p. 624 - 633 Title/Abstract Full Text View citing articles Show Details



Science of Synthesis Search Results after searching Taxol as a full-text term

The screenshot shows the Science of Synthesis search results page. The header includes the Thieme logo and navigation tabs: Home, Query, Results (selected), Full text, and Explore contents. A MySOS user icon is visible in the top right. On the left, a 'REFINE' sidebar shows 'RETRIEVE:' with 'Title (2)' and 'Full text (47)' selected, and 'SORT HITLIST:' with 'By relevance' selected. Below this is an 'Update' button and a 'FUNCTIONS' section with options to 'Select all hits', 'Deselect all hits', and 'Reset all hits'. The main 'Results' section is titled 'Results (Articles Found Containing your Search Term, Structure or Reaction)'. It features a pagination control showing 'Page: 1' and '# 10'. Three search results are displayed, each with a checkbox, a title, a citation, a brief description, and links for 'Show Full text' and 'Show TOC'. The first result is '27.9.1.2.8 Method 8: Taxol A-Ring Side Chain' by Fišera, L. (2004). The second is '20.5.11.1.2.3.3 Variation 3: Synthesis of the Taxol Side Chain Using the Sharpless Catalytic Asymmetric Aminohydroxylation of Cinnamate Esters' by Chemler, S. R.; Zabawa, T. P. (2007). The third is '47.1.3.1.1.4 Method 4: Synthetic Applications of Diels-Alder Reactions' by Fringuelli, F.; Piermatti, O.; Pizzo, F.; Vaccaro, L. (2010).

Thieme Science of Synthesis

Home Query **Results** Full text Explore contents MySOS

REFINE

RETRIEVE:

- Title (2)
- Full text (47)

SORT HITLIST:

- By relevance
- By publication date

Update

FUNCTIONS

- > Select all hits
- > Deselect all hits
- > Reset all hits

Results (Articles Found Containing your Search Term, Structure or Reaction)

Page: 1 # 10

- 27.9.1.2.8 Method 8: Taxol A-Ring Side Chain** #1 of 47
Fišera, L., *Science of Synthesis*, (2004) 27, 359.
Method 8: **Taxol** A-Ring Side Chain
The **taxol** A-ring side chain can be constructed enantioselectively through a thermal, chiral-auxiliary-mediated...
> Show Full text > Show TOC
- 20.5.11.1.2.3.3 Variation 3: Synthesis of the Taxol Side Chain Using the Sharpless Catalytic Asymmetric Aminohydroxylation of Cinnamate Esters** #2 of 47
Chemler, S. R.; Zabawa, T. P., *Science of Synthesis*, (2007) 20, 1224.
Variation 3: Synthesis of the **Taxol** Side Chain Using the Sharpless Catalytic Asymmetric Aminohydroxylation of Cinnamate Esters
...of the most important 2-hydroxyalkanoates is the **taxol** side...
> Show Full text > Show TOC
- 47.1.3.1.1.4 Method 4: Synthetic Applications of Diels-Alder Reactions** #3 of 47
Fringuelli, F.; Piermatti, O.; Pizzo, F.; Vaccaro, L., *Science of Synthesis*, (2010) 47, 655.
s strategy for the synthesis of **taxol** is based on joining the two cyclohexenoids, which represent the rings A and C of **taxol**.
> Show Full text > Show TOC

NAVIGATION

Hit 1 of 47

Previous / Next

27.9.1.2.8 Method 8: Taxol A-Ring Side Chain

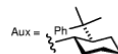
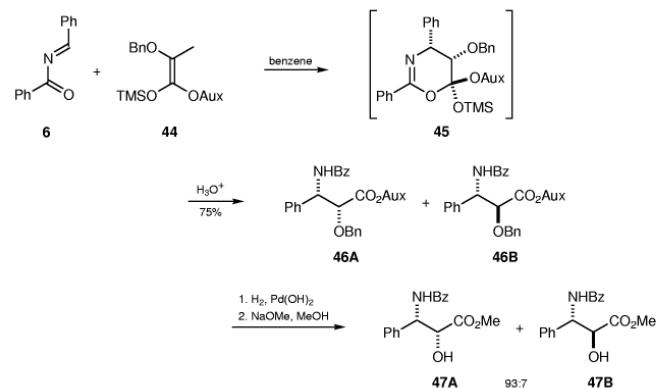
DOI: 10.1055/sos-SD-027-00352



Fišera, L., *Science of Synthesis*, (2004) **27**, 359.

Dihydrooxazines such as **47** can arise from inverse-electron-demand hetero-Diels–Alder reactions.^[30] The **taxol** A-ring side chain can be constructed enantioselectively through a thermal, chiral-auxiliary-mediated variant of this cycloaddition.^[31] Chiral-auxiliary-modified ketene acetal **44** and *N*-acylimine **6** are combined at room temperature to give a mixture of *cis/trans*-dihydrooxazine **45**, which are not isolated. After aqueous acid workup of the cycloaddition mixtures, *syn*- and *anti*-diastereomers **46A** and **46B** are obtained in a 75% combined yield. For the removal of the chiral auxiliary, the mixture of **46A** and **46B** is sequentially debenzylated by catalytic hydrogenation (quantitative) and transesterified with sodium methoxide in methanol (82%) to afford the **taxol** A-ring side chain methyl ester **47A** and the analogous *anti*-methyl ester diastereomer **47B** in a ratio of 93:7 (Scheme 18).

Scheme 18 Preparation of **taxol** A-Ring Side Chain^[31]



References

- [30] Weinreb, S. M.; Scola, P. M., *Chem. Rev.*, (1989) **89**, 1525.
 [31] Swindell, C. S.; Tao, M., *J. Org. Chem.*, (1993) **58**, 5889.

Science of
Synthesis –
first hit in
search results

xSearch Results on Sodium Azide cont.

Committee on Prudent Practices for Handling, Storage, and Disposal of Chemicals in Laboratories, National Research Council
Prudent Practices in the Laboratory - Handling and Disposal of Chemicals
1995-01-01



3 sodium azide



Knovel

...S47Last Update: Jan. 1999 **sodium azide** NaN₃ N₃Na Mol. Wt.: 65.01 CAS Registry No.: 26628-22-8 Synonyms: Nemazyd; Smite EINECS No.: 247-852-1 RTECS No.: VY 8050000 Uses In organic syntheses. Preparation of hydrazoic acid, lead **azide**, pure **sodium**. Differential selection of bacteria. Preservative. Propellant for automotive safety bags. Nematicide. Herbicide. Physical...

Gangolli, S.

Dictionary of Substances and Their Effects (DOSE, 3rd Electronic Edition)

2005-01-01



4 Sodium Azide



Knovel

...Substances Fact Sheet: **Sodium** Arsenite, Trenton, NJ (March 2002) **Sodium azide** S:0390 Molecular Formula: N₃Na Common Formula: NaN₃ Synonyms: AI3-50436; Axiom; Azida sodico (Spanish); **Azide**; Azium; Azoture de **sodium** (French); Dazoe; Hydrazoic acid, **Sodium** salt; Kazoe; Natriumazid (German); NCI-C06462; Smite; **Sodium** salt of hydrazoic acid CAS Registry Number: 26628-22-8;...

Pohanish, Richard P.

Sittig's Handbook of Toxic and Hazardous Chemicals and Carcinogens (5th Edition)

2008-01-01

xSearch – Tentative List of Resources

ACToR (Aggregated Computational Toxicology Resource)

CAMEO Chemicals

Canadian Centre for Occupational Health and Safety. Web Information Service.

Chemical Safety Database

ChemID Plus Advanced

e-EROS : Encyclopedia of Reagents for Organic Synthesis - Chemical Name

Emergency Response Safety and Health Database

Hazardous Substances Data Bank

INCHEM

International Chemical Safety Cards (ICSC) database

Knovel

MSDSonline

NIOSH Pocket Guide to Chemical Hazards

Organic Reactions

Organic Syntheses

PubChem - Compound Search

Science of Synthesis

WebWISER-Known Substance List

Lab Safety Research Guide

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* Electrical safety

* Laser safety

* Lab design

Handling & storage

* Standard operating procedures

* Biological materials

* Hazardous substances

* Reactive substances

* Reagents & solvents

* Nanomaterials

* Waste management

* Spills & emergencies

* Lessons learned

Undergrad lab safety

Websites (Organizations)

Find chemical safety data

Find reactions & protocols

Find safety articles & books

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- Lab Safety Research Guide: <http://library.stanford.edu/guides/lab-safety>
- The Safety Zone by C&EN: <http://cenblog.org/the-safety-zone/>
- ACS Division of Chemical Health & Safety: <http://www.dchas.org/>
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<http://www.acs.org/content/acs/en/about/governance/committees/chemicalsafety.html>
- ACS Committee on Professional Training:
<http://www.acs.org/content/acs/en/about/governance/committees/training.html>

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Stanford Environmental Health and Safety

Stanford Chemistry Department Safety Committee and
Chemistry Department Lab Group Safety Coordinators

