



MATERIAL SAFETY DATA SHEET

according to the Global Harmonized System

Date of issue: 02/04/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number 841522
Product name 1-Ethynylcyclohexanol for synthesis

Relevant identified uses of the substance or mixture and uses advised against

Identified uses Chemical for synthesis

Details of the supplier of the safety data sheet

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United States of America | SDS Phone Support: +1-978-715-1335 |
General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to
4:00 PM Eastern Time (GMT-5)

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Emergency telephone 613-996-6666 CANUTEC (Canada)
+1-703-527-3887 CHEMTREC (International)
24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

Acute toxicity, Category 3, Dermal, H311
Acute toxicity, Category 4, Oral, H302
Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms



Signal Word
Danger

Hazard Statements

H302 Harmful if swallowed.
H311 Toxic in contact with skin.

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H319 Causes serious eye irritation.

Precautionary Statements

P280 Wear protective gloves/ protective clothing.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	C ₈ H ₁₂ O (Hill)
CAS-No.	78-27-3
Molar mass	124.18 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

1-Ethynylcyclohexanol (>= 90 % - <= 100 %)

78-27-3

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Consult doctor if feeling unwell.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing. Call a physician immediately.

Eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

Ingestion

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Cough, Shortness of breath, Drowsiness, Dizziness, narcosis, Diarrhea, Nausea, Vomiting, drowsiness

Indication of any immediate medical attention and special treatment needed

No information available.

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SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible material, Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapors possible in the event of fire.

Fire may cause evolution of:

Acetylene

Advice for firefighters

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of vapors/aerosols or dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Depending on the state of matter, take up with suitable equipment or with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store at +15°C to +25°C (+59°F to +77°F).

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SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

protective clothing

Respiratory protection

required when dusts/vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	solid
Color	colorless
Odor	characteristic odor
Odor Threshold	No information available.
pH	7 at 1 g/l 68 °F (20 °C)
Melting point	30 - 32 °C
Boiling point/boiling range	356 °F (180 °C) at 1,013 hPa

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Flash point	163 °F (73 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1.3 %(V)
Upper explosion limit	8.7 %(V)
Vapor pressure	1 hPa at 122 °F (50 °C)
Relative vapor density	3.7
Relative density	0.976 g/cm ³ at 68 °F (20 °C)
Water solubility	10 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 1.73 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	689 °F (365 °C)

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong reducing agents, Strong acids, strong alkalis, Acid anhydrides, acid halides, Heavy metal salts

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Conditions to avoid

Strong heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Incompatible materials

no information available

Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 583 mg/kg (RTECS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Nausea, Vomiting
absorption

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 rabbit: 973 mg/kg
(RTECS)

absorption

Skin irritation

rabbit

Result: No irritation

OECD Test Guideline 404

Eye irritation

rabbit

Result: Eye irritation

OECD Test Guideline 405

Causes serious eye irritation.

Genotoxicity in vitro

Ames test

Result: negative

(External MSDS)

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

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Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

After absorption of toxic quantities:

Systemic effects:

Cough, Drowsiness, drowsiness, Diarrhea, Dizziness, narcosis

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 *Leuciscus idus* (Golden orfe): > 220 - 460 mg/l; 96 h (External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia*: 160 mg/l; 48 h (External MSDS)

Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): > 500 mg/l; 72 h (External MSDS)

Toxicity to bacteria

EC50 *Pseudomonas putida*: 1,800 mg/l; 17 h (External MSDS)

Persistence and degradability

Biodegradability

20 - 70 %

OECD Test Guideline 302B

Moderately (partly) eliminable (DOC reduction 20-70 %).

Biochemical Oxygen Demand (BOD)

3 mg/g

(External MSDS)

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Chemical Oxygen Demand (COD)

2,750 mg/g
(External MSDS)

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1.73
(experimental)
(Lit.) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 2811
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (1-ETHYNYLCYCLOHEXANOL)
Class	6.1
Packing group	III
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 2811
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (1-ETHYNYLCYCLOHEXANOL)
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 2811
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (1-ETHYNYLCYCLOHEXANOL)
Class	6.1
Packing group	III

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Environmentally hazardous --
Special precautions for user yes
EmS F-A S-A

SECTION 15. Regulatory information

United States of America

Canada

WHMIS Classification

D1B Toxic Material Causing Immediate and Serious Toxic Effects

D2B Toxic Material Causing Other Toxic Effects

Toxic by skin absorption, Eye irritant

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

Notification status

TSCA: On TSCA Inventory

DSL: This product contains one or several components listed in the
Canadian NDSL.

Ingredients

1-Ethynylcyclohexanol

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Full text of H-Statements referred to under sections 2 and 3.

H302 Harmful if swallowed.

H311 Toxic in contact with skin.

H319 Causes serious eye irritation.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Date of issue: 02/04/2013

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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