

# Safety Data Sheet

acc. to OSHA HCS

Printing date 05/22/2024

Reviewed on 05/22/2024

## 1 Identification

- **Product identifier**
- **Trade name:** 2% Allyl Alcohol; 2%1-propanol  
2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w
- **Article number:** MOT092
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**  
Aqua Solutions, Inc.  
6913 Highway 225  
DEER PARK, TX 77536  
USA  
800-256-2586
- **Information department:**  
Technical Coordinator  
Sherman Nelson [shermann@aquasolutions.org](mailto:shermann@aquasolutions.org)  
Technical Coordinator  
Sherman Nelson [shermann@aquasolutions.org](mailto:shermann@aquasolutions.org)
- **Emergency telephone number:**  
Chemtrec: 800-424-9300  
Canutec: 613-996-6666



## 2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS02 Flame

Flammable Liquids 2      H225 Highly flammable liquid and vapor.



GHS06 Skull and crossbones

Acute Toxicity - Dermal 3      H311 Toxic in contact with skin.



GHS08 Health hazard

Carcinogenicity 2      H351 Suspected of causing cancer.



GHS07

Acute Toxicity - Oral 4      H302 Harmful if swallowed.

Acute Toxicity - Inhalation 4      H332 Harmful if inhaled.

Eye Irritation 2A      H319 Causes serious eye irritation.

- **Label elements**
- **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).

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**Trade name:** 2% Allyl Alcohol; 2% 1-propanol  
2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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· **Hazard pictograms**



GHS02   GHS06   GHS07   GHS08

· **Signal word** *Danger*

· **Hazard-determining components of labeling:**

Acetonitrile, Reagent ACS Grade

4-Vinyl-1-Cyclohexene

allyl alcohol

n-propanol

· **Hazard statements**

Highly flammable liquid and vapor.

Harmful if swallowed or if inhaled.

Toxic in contact with skin.

Causes serious eye irritation.

Suspected of causing cancer.

· **Precautionary statements**

Obtain special instructions before use.

Do not handle until all safety precautions have been read and understood.

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Keep container tightly closed.

Ground/bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

Take precautionary measures against static discharge.

Avoid breathing dust/fume/gas/mist/vapors/spray

Wash thoroughly after handling.

Do not eat, drink or smoke when using this product.

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection.

If swallowed: Call a poison center/doctor if you feel unwell.

Rinse mouth.

If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continue rinsing.

IF exposed or concerned: Get medical advice/attention.

Specific treatment (see on this label).

Take off immediately all contaminated clothing and wash it before reuse.

If eye irritation persists: Get medical advice/attention.

In case of fire: Use CO<sub>2</sub>, powder or water spray to extinguish.

Store in a well-ventilated place. Keep cool.

Store locked up.

Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Classification system:**

· **NFPA ratings (scale 0 - 4)**



Health = 2

Fire = 3

Reactivity = 0

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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· **HMIS-ratings (scale 0 - 4)**

HEALTH	2	Health = *2
FIRE	3	Fire = 3
REACTIVITY	0	Reactivity = 0

- **Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

### 3 Composition/information on ingredients

- **Chemical characterization:** Mixtures
- **Description:** Mixture of the substances listed below with nonhazardous additions.

· **Dangerous components:**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	94.0%
CAS: 71-23-8	n-propanol	2.0%
CAS: 100-40-3	4-Vinyl-1-Cyclohexene	2.0%
CAS: 107-18-6	allyl alcohol	2.0%

### 4 First-aid measures

- **Description of first aid measures**
- **General information:**  
Immediately remove any clothing soiled by the product.  
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.  
In case of irregular breathing or respiratory arrest provide artificial respiration.
- **After inhalation:**  
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.  
In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:**  
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
- **After swallowing:** Immediately call a doctor.
- **Information for doctor:**  
· **Most important symptoms and effects, both acute and delayed** No further relevant information available.  
· **Indication of any immediate medical attention and special treatment needed**  
No further relevant information available.

### 5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**  
CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture** No further relevant information available.

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**Trade name:** 2% Allyl Alcohol; 2%1-propanol  
2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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- **Advice for firefighters**
- **Protective equipment:** Mouth respiratory protective device.

## 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**  
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:**  
Do not allow product to reach sewage system or any water course.  
Inform respective authorities in case of seepage into water course or sewage system.  
Dilute with plenty of water.  
Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**  
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).  
Dispose contaminated material as waste according to section 13.  
Ensure adequate ventilation.
- **Reference to other sections**  
See Section 7 for information on safe handling.  
See Section 8 for information on personal protection equipment.  
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**

- **PAC-1:**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	13 ppm
CAS: 71-23-8	n-propanol	250 ppm
CAS: 100-40-3	4-Vinyl-1-Cyclohexene	0.3 ppm
CAS: 107-18-6	allyl alcohol	0.09 ppm

- **PAC-2:**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	50 ppm
CAS: 71-23-8	n-propanol	670 ppm
CAS: 100-40-3	4-Vinyl-1-Cyclohexene	210 ppm
CAS: 107-18-6	allyl alcohol	1.7 ppm

- **PAC-3:**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	150 ppm
CAS: 71-23-8	n-propanol	4000* ppm
CAS: 100-40-3	4-Vinyl-1-Cyclohexene	340 ppm
CAS: 107-18-6	allyl alcohol	13 ppm

## 7 Handling and storage

- **Handling:**
- **Precautions for safe handling**  
Ensure good ventilation/exhaustion at the workplace.  
Open and handle receptacle with care.  
Prevent formation of aerosols.
- **Information about protection against explosions and fires:**  
Keep ignition sources away - Do not smoke.  
Protect against electrostatic charges.

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w**

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Keep respiratory protective device available.

- **Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** Store in a cool location.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:**  
Keep receptacle tightly sealed.  
Store in cool, dry conditions in well sealed receptacles.
- **Specific end use(s)** No further relevant information available.

## 8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see section 7.
- **Control parameters**

· **Components with limit values that require monitoring at the workplace:**

**CAS: 75-05-8 Acetonitrile, Reagent ACS Grade**

PEL Long-term value: 70 mg/m<sup>3</sup>, 40 ppm

REL Long-term value: 34 mg/m<sup>3</sup>, 20 ppm

TLV Long-term value: 20 ppm  
Skin, A4

**CAS: 71-23-8 n-propanol**

PEL Long-term value: 500 mg/m<sup>3</sup>, 200 ppm

REL Short-term value: 625 mg/m<sup>3</sup>, 250 ppm  
Long-term value: 500 mg/m<sup>3</sup>, 200 ppm  
Skin

TLV Long-term value: 100 ppm  
A4

**CAS: 100-40-3 4-Vinyl-1-Cyclohexene**

TLV Long-term value: 0.1 ppm  
A3

WEEL Long-term value: 4.4 mg/m<sup>3</sup>, 1 ppm

**CAS: 107-18-6 allyl alcohol**

PEL Long-term value: 5 mg/m<sup>3</sup>, 2 ppm  
Skin

REL Short-term value: 10 mg/m<sup>3</sup>, 4 ppm  
Long-term value: 5 mg/m<sup>3</sup>, 2 ppm  
Skin

TLV Long-term value: 0.5 ppm  
Skin, A4

· **Additional information:** The lists that were valid during the creation were used as basis.

- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**  
Keep away from foodstuffs, beverages and feed.  
Immediately remove all soiled and contaminated clothing.  
Wash hands before breaks and at the end of work.

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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Store protective clothing separately.

Avoid contact with the eyes.

Avoid contact with the eyes and skin.

· **Breathing equipment:**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

· **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

· **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

· **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

· **Eye protection:**



Tightly sealed goggles

· **Body protection:** Protective work clothing

## 9 Physical and chemical properties

· **Information on basic physical and chemical properties**

· **General Information**

· **Appearance:**

Form: Liquid

Color: Clear

· **Odor:** Characteristic

· **Odor threshold:** Not determined.

· **pH-value:** Not determined.

· **Change in condition**

Melting point/Melting range: Undetermined.

Boiling point/Boiling range: Undetermined.

· **Flash point:** 5 °C (41 °F)

· **Flammability (solid, gaseous):** Highly flammable.

· **Auto igniting:** 525 °C (977 °F)

· **Decomposition temperature:** Not determined.

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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· <b>Ignition temperature:</b>	Product is not selfigniting.
· <b>Danger of explosion:</b>	Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
· <b>Explosion limits:</b>	
<b>Lower:</b>	4.4 Vol %
<b>Upper:</b>	16 Vol %
· <b>Vapor pressure at 20 °C (68 °F):</b>	97 hPa (72.8 mm Hg)
· <b>Density at 20 °C (68 °F):</b>	0.78498 g/cm <sup>3</sup> (6.55066 lbs/gal)
· <b>Relative density</b>	Not determined.
· <b>Vapor density</b>	Not determined.
· <b>Evaporation rate</b>	Not determined.
· <b>Solubility in / Miscibility with Water:</b>	Fully miscible.
· <b>Partition coefficient (n-octanol/water):</b>	Not determined.
· <b>Viscosity:</b>	
<b>Dynamic:</b>	Not determined.
<b>Kinematic:</b>	Not determined.
· <b>Solvent content:</b>	
<b>Organic solvents:</b>	4.0 %
<b>VOC content:</b>	4.00 %
	31.4 g/l / 0.26 lb/gal
<b>Solids content:</b>	0.0 %
· <b>Other information</b>	No further relevant information available.

## 10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

## 11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**

· <b>LD/LC50 values that are relevant for classification:</b>		
<b>ATE (Acute Toxicity Estimate)</b>		
Oral	LD50	454 mg/kg
Dermal	LD50	770 mg/kg
Inhalative	LC50/4h	10.9 mg/l

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**Trade name:** 2% Allyl Alcohol; 2%1-propanol  
2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

(Contd. of page 7)

- **Primary irritant effect:**
- **on the skin:** No irritant effect.
- **on the eye:** Irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**

The product shows the following dangers according to internally approved calculation methods for preparations:

Toxic

Harmful

Irritant

- **Carcinogenic categories**

- **IARC (International Agency for Research on Cancer)**

CAS: 100-40-3 4-Vinyl-1-Cyclohexene

2B

- **NTP (National Toxicology Program)**

None of the ingredients is listed.

- **OSHA-Ca (Occupational Safety & Health Administration)**

None of the ingredients is listed.

## 12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**
- Water hazard class 2 (Self-assessment): hazardous for water
- Do not allow product to reach ground water, water course or sewage system.
- Danger to drinking water if even small quantities leak into the ground.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

## 13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
- Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.
- **Recommended cleansing agent:** Water, if necessary with cleansing agents.

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w

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## 14 Transport information

<ul style="list-style-type: none"> <li>· UN-Number</li> <li>· DOT, IMDG, IATA</li> </ul>	UN1993
<ul style="list-style-type: none"> <li>· UN proper shipping name</li> <li>· DOT</li> <li>· IMDG, IATA</li> </ul>	<p>Flammable liquids, n.o.s. (acetonitrile, allyl alcohol, n-propanol, 4-Vinyl-1-Cyclohexene)</p> <p>FLAMMABLE LIQUID, N.O.S. (acetonitrile, allyl alcohol, n-propanol, 4-Vinyl-1-Cyclohexene)</p>
<ul style="list-style-type: none"> <li>· Transport hazard class(es)</li> <li>· DOT</li> </ul>	<div style="text-align: center;">  </div>
<ul style="list-style-type: none"> <li>· Class</li> <li>· Label</li> </ul>	<p>3 Flammable liquids</p> <p>3</p>
<ul style="list-style-type: none"> <li>· IMDG, IATA</li> </ul>	<div style="text-align: center;">  </div>
<ul style="list-style-type: none"> <li>· Class</li> <li>· Label</li> </ul>	<p>3 Flammable liquids</p> <p>3</p>
<ul style="list-style-type: none"> <li>· Packing group</li> <li>· DOT, IMDG</li> <li>· IATA</li> </ul>	<p>II</p> <p>I</p>
<ul style="list-style-type: none"> <li>· Environmental hazards:</li> <li>· Marine pollutant:</li> </ul>	<p>No</p>
<ul style="list-style-type: none"> <li>· Special precautions for user</li> <li>· Hazard identification number (Kemler code):</li> <li>· EMS Number:</li> <li>· Stowage Category</li> </ul>	<p>Warning: Flammable liquids</p> <p>336</p> <p>F-E, S-E</p> <p>B</p>
<ul style="list-style-type: none"> <li>· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</li> </ul>	<p>Not applicable.</p>
<ul style="list-style-type: none"> <li>· Transport/Additional information:</li> <li>· DOT</li> <li>· Quantity limitations</li> </ul>	<p>On passenger aircraft/rail: 1 L</p> <p>On cargo aircraft only: 30 L</p>
<ul style="list-style-type: none"> <li>· IMDG</li> <li>· Limited quantities (LQ)</li> <li>· Excepted quantities (EQ)</li> </ul>	<p>0</p> <p>Code: E3</p> <p>Maximum net quantity per inner packaging: 30 ml</p> <p>Maximum net quantity per outer packaging: 300 ml</p>

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2% 4-Vinyl-1-Cyclohexene in Acetonitrile w/w

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· **UN "Model Regulation":** UN 1993 FLAMMABLE LIQUID, N.O.S. (ACETONITRILE, ALLYL ALCOHOL, N-PROPANOL, 4-VINYL-1-CYCLOHEXENE), 3, II

## 15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**  
No further relevant information available.

· **Sara**

· **Section 355 (extremely hazardous substances):**

CAS: 107-18-6	allyl alcohol
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· **Section 313 (Specific toxic chemical listings):**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade
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CAS: 107-18-6	allyl alcohol
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· **TSCA (Toxic Substances Control Act):**

Acetonitrile, Reagent ACS Grade	ACTIVE
n-propanol	ACTIVE
4-Vinyl-1-Cyclohexene	ACTIVE
allyl alcohol	ACTIVE

· **Hazardous Air Pollutants**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade
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· **Proposition 65**

· **Chemicals known to cause cancer:**

CAS: 100-40-3	4-Vinyl-1-Cyclohexene
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· **Chemicals known to cause reproductive toxicity for females:**

CAS: 100-40-3	4-Vinyl-1-Cyclohexene
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· **Chemicals known to cause reproductive toxicity for males:**

None of the ingredients is listed.

· **Chemicals known to cause developmental toxicity:**

None of the ingredients is listed.

· **Carcinogenic categories**

· **EPA (Environmental Protection Agency)**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	CBD, D
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· **TLV (Threshold Limit Value)**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	A4
CAS: 71-23-8	n-propanol	A4
CAS: 100-40-3	4-Vinyl-1-Cyclohexene	A3
CAS: 107-18-6	allyl alcohol	A4

· **NIOSH-Ca (National Institute for Occupational Safety and Health)**

None of the ingredients is listed.

· **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).

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· **Hazard pictograms**



GHS02   GHS06   GHS07   GHS08

· **Signal word** *Danger*

· **Hazard-determining components of labeling:**

Acetonitrile, Reagent ACS Grade

4-Vinyl-1-Cyclohexene

allyl alcohol

n-propanol

· **Hazard statements**

Highly flammable liquid and vapor.

Harmful if swallowed or if inhaled.

Toxic in contact with skin.

Causes serious eye irritation.

Suspected of causing cancer.

· **Precautionary statements**

Obtain special instructions before use.

Do not handle until all safety precautions have been read and understood.

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Keep container tightly closed.

Ground/bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

Take precautionary measures against static discharge.

Avoid breathing dust/fume/gas/mist/vapors/spray

Wash thoroughly after handling.

Do not eat, drink or smoke when using this product.

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection.

If swallowed: Call a poison center/doctor if you feel unwell.

Rinse mouth.

If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continue rinsing.

IF exposed or concerned: Get medical advice/attention.

Specific treatment (see on this label).

Take off immediately all contaminated clothing and wash it before reuse.

If eye irritation persists: Get medical advice/attention.

In case of fire: Use CO<sub>2</sub>, powder or water spray to extinguish.

Store in a well-ventilated place. Keep cool.

Store locked up.

Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

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2% 4-Vinyl 1-Cyclohexene in Acetonitrile w/w**

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## 16 Other information

*This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.*

· **Department issuing SDS:** Environment protection department.

· **Contact:**

*Date of Preparation / Last Revision:*

· **Date of preparation / last revision**

*Revision 1.2, 05/21/2024: Reviewed SDS for accuracy. MH/STN*

*Creation date for SDS 12-03-2014. STN*

*05/22/2024*

· **Abbreviations and acronyms:**

*IMDG: International Maritime Code for Dangerous Goods*

*DOT: US Department of Transportation*

*IATA: International Air Transport Association*

*EINECS: European Inventory of Existing Commercial Chemical Substances*

*ELINCS: European List of Notified Chemical Substances*

*CAS: Chemical Abstracts Service (division of the American Chemical Society)*

*NFPA: National Fire Protection Association (USA)*

*HMIS: Hazardous Materials Identification System (USA)*

*VOC: Volatile Organic Compounds (USA, EU)*

*LC50: Lethal concentration, 50 percent*

*LD50: Lethal dose, 50 percent*

*PBT: Persistent, Bioaccumulative and Toxic*

*vPvB: very Persistent and very Bioaccumulative*

*NIOSH: National Institute for Occupational Safety*

*OSHA: Occupational Safety & Health*

*TLV: Threshold Limit Value*

*PEL: Permissible Exposure Limit*

*REL: Recommended Exposure Limit*

*Flammable Liquids 2: Flammable liquids – Category 2*

*Acute Toxicity - Oral 4: Acute toxicity – Category 4*

*Acute Toxicity - Dermal 3: Acute toxicity – Category 3*

*Eye Irritation 2A: Serious eye damage/eye irritation – Category 2A*

*Carcinogenicity 2: Carcinogenicity – Category 2*

· **\* Data compared to the previous version altered.**

US