

• SAFETY DATA SHEET

Version 6.9
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : N-Vinylcaprolactam
Product Number : 415464
Brand : Aldrich
CAS-No. : 2235-00-9

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

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

Acute toxicity (Dermal) : Category 4
Eye irritation : Category 2A
Skin sensitisation : Category 1
Specific target organ toxicity - repeated exposure : Category 1 (Liver, Upper respiratory tract)

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H302 + H312 Harmful if swallowed or in contact with skin.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H372 Causes damage to organs (Liver, Upper respiratory tract) through prolonged or repeated exposure.

Precautionary statements : **Prevention:**
P260 Do not breathe dust.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P272 Contaminated work clothing must not be allowed out of the workplace.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 + P312 IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314 Get medical advice/ attention if you feel unwell.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical

advice/ attention.
P363 Wash contaminated clothing before reuse.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 2235-00-9

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
1-vinylhexahydro-2H-azepin-2-one	2235-00-9*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : Show this safety data sheet to the doctor in attendance.
- If inhaled : After inhalation: fresh air. Call in physician.
- In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
- In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
- If swallowed : After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.
- Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

Specific extinguishing methods : No data available

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

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Avoid generation and inhalation of dusts in all circumstances.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:

Aldrich - 415464

Page 4 of 13

For personal protection see section 8.

- Environmental precautions : Do not let product enter 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).
Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
- Further information on storage conditions : Tightly closed.
Dry.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
- Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection

Aldrich - 415464

Page 5 of 13

Remarks	: Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.
Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	: protective clothing
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: solid
Color	: off-white
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: 262 °F / 128 °C (28 hPa) Method: lit.
Flash point	: 214 °F / 101 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available

Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: 6.5 %(V)
Lower explosion limit / Lower flammability limit	: 1.4 %(V)
Vapor pressure	: < 0.1 mbar (68 °F / 20 °C) 1.6 mbar (158 °F / 70 °C)
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.029 g/cm ³ (77 °F / 25 °C) Method: lit.
Solubility(ies) Water solubility	: ca. 4.1 g/l
Partition coefficient: n- octanol/water	: log Pow: 1.2
Autoignition temperature	: 428 °F / 220 °C
Decomposition temperature	: No data available
Viscosity Viscosity, dynamic	: No data available
Viscosity, kinematic	: 6.16 mm ² /s (68 °F / 20 °C) 3.50 mm ² /s (104 °F / 40 °C)
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 139.19 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical. 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	: Stable under recommended storage conditions.
Conditions to avoid	: Heat Strong heating.
Incompatible materials	: acids Oxidizing agents Polymerizing initiators Free radical initiators
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - 500.1 mg/kg

Inhalation: No data available

Dermal: No data available

LD50 Dermal - Rabbit - male and female - 1,700 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

Respiratory or skin sensitization

in vivo assay - Mouse

Result: May cause sensitisation by skin contact.
(OECD Test Guideline 429)

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

The substance or mixture is classified as specific target organ toxicant, repeated exposure, category 1.

- Liver, Upper respiratory tract

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

1-vinylhexahydro-2H-azepin-2-one:

Toxicity to fish : LC50 (Brachydanio rerio (zebrafish)): 318 mg/l
Exposure time: 96 h
Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates : (Daphnia magna (Water flea)): > 100 mg/l
Exposure time: 48 h

Toxicity to algae/aquatic plants : EC50 (Desmodesmus subspicatus (green algae)): > 100 mg/l
Exposure time: 72 h

Persistence and degradability

Components:

1-vinylhexahydro-2H-azepin-2-one:

Biodegradability : Result: Readily biodegradable.

Bioaccumulative potential

Components:

1-vinylhexahydro-2H-azepin-2-one:

Bioaccumulation : Remarks: No bioaccumulation is to be expected (log Pow <= 4).

Partition coefficient: n-octanol/water : log Pow: 1.2

Mobility in soil

Components:

1-vinylhexahydro-2H-azepin-2-one:

Stability in soil : Remarks: No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

1-vinylhexahydro-2H-azepin-2-one:

Additional ecological information : No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

Aldrich - 415464

Page 10 of 13

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations**49 CFR Road**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION**CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

1-vinylhexahydro-2H-azepin-2-one

2235-00-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory;

Aldrich - 415464

Page 12 of 13

LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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