SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: ε-Caprolactam
Product Number: C2204
Brand: Aldrich
Index-No.: 613-069-00-2
CAS-No.: 105-60-2

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

Identified uses: Laboratory chemicals, Synthesis of substances

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

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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

2.2 GHS Label elements, including precautionary statements
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

Pictogram

Signal Word

Warning

Hazard statement(s)
H302 + H332 Harmful if swallowed or if inhaled.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

Precautionary statement(s)
P261 Avoid breathing dust.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. 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.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms:
- Aza-2-cycloheptanone
- 2-Oxohexamethyleneimine
- epsilon-Caprolactam

Formula: \( \text{C}_6\text{H}_{11}\text{NO} \)
Molecular weight: 113.16 g/mol
CAS-No.: 105-60-2
EC-No.: 203-313-2
Index-No.: 613-069-00-2

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varepsilon )-caprolactam</td>
<td>Acute Tox. 4; Skin Irrit. 2;</td>
<td>( \leq 100% )</td>
</tr>
</tbody>
</table>

Aldrich - C2204

Page 2 of 11
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

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

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

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

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Combustible.
Vapors 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.
5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **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

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains.

6.3 **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.

6.4 **Reference to other sections**
For disposal see section 13.

SECTION 7: Handling and storage

7.1 **Precautions for safe handling**

**Advice on safe handling**
Work under hood. Do not inhale substance/mixture.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Tightly closed. Dry.

Hygroscopic

**Storage class**
Storage class (TRGS 510): 11: Combustible Solids

7.3 **Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated
SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>ε-caprolactam</td>
<td>105-60-2</td>
<td>TWA 5 mg/m3</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td>Remarks</td>
<td></td>
<td></td>
<td>Not suspected as a human carcinogen</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>Control parameters</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Basis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td>1 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ST</td>
<td>3 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td>0.22 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ST</td>
<td>0.66 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PEL</td>
<td>1 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PEL</td>
<td>5 ppm 20 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>STEL</td>
<td>3 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>STEL</td>
<td>10 ppm 40 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
Recommended Filter type: Filter A-(P2)
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

**Control of environmental exposure**
Do not let product enter drains.

---

**SECTION 9: Physical and chemical properties**

9.1 Information on basic physical and chemical properties

| a) Appearance | Form: crystalline |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | 7.0 - 8.5 at 333 g/l |
| e) Melting point/freezing point | Melting point/range: 68 - 71 °C (154 - 160 °F) - lit. |
| f) Initial boiling point and boiling range | 136 - 138 °C 277 - 280 °F at 13 hPa - lit. |
| g) Flash point | 152 °C (306 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower | Upper explosion limit: 11.9 % (V) |
flammbility or explosive limits  Lower explosion limit: 1.6 % (V)

k) Vapor pressure  9 hPa at 60 °C (140 °F)  
< 0.01 hPa at 20 °C (68 °F)

l) Vapor density  No data available

m) Density  1.020 g/cm³ at 75 °C (167 °F)
Relative density  No data available

n) Water solubility  soluble

o) Partition coefficient:  
n-octanol/water  log Pow: 0.12 at 25 °C (77 °F)

p) Autoignition temperature  No data available

q) Decomposition temperature  No data available

r) Viscosity  No data available

s) Explosive properties  No data available

t) Oxidizing properties  No data available

9.2 Other safety information  
No data available

SECTION 10: Stability and reactivity

10.1 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.

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

10.3 Possibility of hazardous reactions  
Risk of explosion with:  
Strong oxidizing agents  
acetic acid  
with  
nitrogen oxides  
Violent reactions possible with:  
alkalines  
acids

10.4 Conditions to avoid  
hygroscopic

Aldrich - C2204
Strong heating.

10.5 Incompatible materials
Strong oxidizing agents

10.6 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 - Rat - 1,210 mg/kg
Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste): Eye: Chromodacryorrhea.
Behavioral: Convulsions or effect on seizure threshold.
Nutritional and Gross Metabolic: Changes in Body temperature decrease.

LC50 Inhalation - Rat - 300 mg/m3

LC50 Inhalation - Mouse - 450 mg/m3
Remarks: Behavioral: Muscle contraction or spasticity.

LD50 Dermal - Rat - > 2,000 mg/kg
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Mild skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Moderate eye irritation - 24 h
Eyes - Rabbit
Result: Moderate eye irritation - 24 h

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
This product is or contains a component that is probably not carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

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.

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.

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

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
RTECS: CM3675000
Convulsions, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological Information

12.1 Toxicity
Toxicity to algae
EC50 - Pseudokirchneriella subcapitata (green algae) - 4,320 - 4,800 mg/l - 72 h
IC50 - Desmodesmus subspicatus (green algae) - 130 mg/l - 72 h
Remarks: (IUCLID)
(ε-caprolactam)

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available
SECTION 13: Disposal considerations

13.1 Waste treatment methods

**Product**
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

**DOT (US)**
Not dangerous goods

**IMDG**
Not dangerous goods

**IATA**
Not dangerous goods

**Further information**
Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

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

**SARA 313 Components**
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.

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>ε-caprolactam</td>
<td>105-60-2</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>ε-caprolactam</td>
<td>105-60-2</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>

Aldrich - C2204

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact misbranding@sial.com.
Version: 6.7 Revision Date: 10/27/2023 Print Date: 01/06/2024