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

1.1 Product identifiers

Product name: Phenylacetylene
Product Number: 117706
Brand: Aldrich
CAS-No.: 536-74-3

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)

- Flammable liquids (Category 3), H226
- Skin irritation (Category 2), H315
- Eye irritation (Category 2A), H319
- Carcinogenicity (Category 1B), H350
- 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

Pictogram

Signal Word: Danger
Hazard statement(s)
H226  Flammable liquid and vapor.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H335  May cause respiratory irritation.
H350  May cause cancer.

Precautionary statement(s)
P201  Obtain special instructions before use.
P202  Do not handle until all safety precautions have been read and understood.
P210  Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233  Keep container tightly closed.
P240  Ground/bond container and receiving equipment.
P241  Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242  Use only non-sparking tools.
P243  Take precautionary measures against static discharge.
P261  Avoid breathing mist or vapors.
P264  Wash skin thoroughly after handling.
P271  Use only outdoors or in a well-ventilated area.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353  IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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.
P308 + P313  IF exposed or concerned: Get medical advice/ attention.
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.
P370 + P378  In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233  Store in a well-ventilated place. Keep container tightly closed.
P403 + P235  Store in a well-ventilated place. Keep cool.
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 : Ethynylbenzene
Acetylene, phenyl-
Phenylacetylene
Phenylacetylide
Phenylethyne
1-Phenylethyne
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

### 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. 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 an 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
Carbon dioxide (CO2) Foam 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
Combustible.
Mixture with combustible ingredients.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
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
Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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**
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage stability**
Recommended storage temperature
2 - 8 °C
Moisture sensitive.

**Storage class**
Storage class (TRGS 510): 3: Flammable liquids

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>1,4-Dioxane</td>
<td>123-91-1</td>
<td>TWA</td>
<td>20 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks
Confirmed animal carcinogen with unknown relevance to humans
Danger of cutaneous absorption

<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>25 ppm</th>
<th>90 mg/m³</th>
<th>USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)</th>
</tr>
</thead>
</table>

Skin notation

<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>100 ppm</th>
<th>360 mg/m³</th>
<th>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</th>
</tr>
</thead>
</table>

Skin designation

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>1 ppm</th>
<th>3.6 mg/m³</th>
<th>USA. NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
</table>

Potential Occupational Carcinogen

<table>
<thead>
<tr>
<th></th>
<th>PEL</th>
<th>0.28 ppm</th>
<th>1 mg/m³</th>
<th>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</th>
</tr>
</thead>
</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
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.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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).

Control of environmental exposure
Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance Form: liquid
b) Odor No data available
c) Odor Threshold No data available
d) pH No data available
e) Melting Melting point: -44.8 °C (-48.6 °F)
point/freezing point
f) Initial boiling point and boiling range 142 - 144 °C 288 - 291 °F

g) Flash point 27 °C (81 °F) - closed cup

h) Evaporation rate No data available

i) Flammability (solid, gas) No data available

j) Upper/lower flammability or explosive limits No data available

k) Vapor pressure 23.4647 hPa at 37.7 °C (99.9 °F)
l) Vapor density No data available

m) Density 0.93 g/mL at 25 °C (77 °F)
   Relative density No data available

n) Water solubility No data available

o) Partition coefficient: n-octanol/water No data available

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
Vapor/air-mixtures are explosive at intense warming.

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

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Oxidizing agents
halogens
Alkali metals
perchloric acid
acids

10.4 Conditions to avoid
Exposure to moisture.
Heat, flames and sparks.
Heating.

10.5 Incompatible materials
No data available

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
Oral: No data available
Inhalation: No data available
Dermal: No data available
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation
(OECD Test Guideline 404)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: styrene

Serious eye damage/eye irritation
Eyes - Rabbit
Result: irritating
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: styrene

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
IARC: 2B - Group 2B: Possibly carcinogenic to humans (1,4-Dioxane)
NTP: RAHC - Reasonably anticipated to be a human carcinogen (1,4-Dioxane)
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
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
RTECS: DA0780000
Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity
No data available

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)
UN number: 3295  Class: 3  Packing group: III
Proper shipping name: Hydrocarbons, liquid, n.o.s.
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 3295  Class: 3  Packing group: III  EMS-No: F-E, S-D
Proper shipping name: HYDROCARBONS, LIQUID, N.O.S.
SECTION 15: Regulatory information

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

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Proper shipping name</th>
<th>CAS-No.</th>
<th>Revision Date</th>
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<td>1,4-Dioxane</td>
<td>123-91-1</td>
<td>2007-07-01</td>
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</table>

Massachusetts Right To Know Components

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Pennsylvania Right To Know Components

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</tbody>
</table>

California Prop. 65 Components

1,4-Dioxane, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov, 1,4-Dioxane

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<tbody>
<tr>
<td>1,4-Dioxane</td>
<td>123-91-1</td>
<td>2007-09-28</td>
</tr>
</tbody>
</table>

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.

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Version: 6.6 Revision Date: 03/17/2023 Print Date: 07/08/2023