1. PRODUCT AND COMPANY IDENTIFICATION

Product name: Phenylacetylene
Product Number: 117706
Brand: Aldrich
Supplier: Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO  63103
USA
Telephone: +1 800-325-5832
Fax: +1 800-325-5052
Emergency Phone #: (314) 776-6555
Preparation Information: Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable liquid, Carcinogen, Target Organ Effect, Irritant

GHS Classification
Flammable liquids (Category 3)
Skin irritation (Category 2)
Eye irritation (Category 2A)
Carcinogenicity (Category 2)
Aspiration hazard (Category 1)

GHS Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s)

H226  Flammable liquid and vapour.
H304  May be fatal if swallowed and enters airways.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H351  Suspected of causing cancer.

Precautionary statement(s)

P281  Use personal protective equipment as required.
P301 + P310  IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P305 + P351 + P338  IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P331  Do NOT induce vomiting.

HMIS Classification

Health hazard: 2
Chronic Health Hazard: *
Flammability: 3
Physical hazards: 0

NFPA Rating
Health hazard: 2
Fire: 3
Reactivity Hazard: 0

Potential Health Effects
Inhalation: May be harmful if inhaled. Causes respiratory tract irritation.
Skin: May be harmful if absorbed through skin. Causes skin irritation.
Eyes: Causes eye irritation.
Ingestion: May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms:
- Ethynylbenzene
- Acetylene, phenyl-
- Phenylacetylene
- Phenylacetylide
- Phenylethyne
- 1-Phenylethyne

Formula: C₈H₆
Molecular Weight: 102.13 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenylacetylene</td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>536-74-3</td>
</tr>
<tr>
<td>EC-No.</td>
<td>208-645-1</td>
</tr>
<tr>
<td></td>
<td>90 100 %</td>
</tr>
<tr>
<td>1,4-Dioxane</td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>123-91-1</td>
</tr>
<tr>
<td>EC-No.</td>
<td>204-661-8</td>
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<tr>
<td>Index-No.</td>
<td>603-024-00-5</td>
</tr>
<tr>
<td></td>
<td>0.11 %</td>
</tr>
</tbody>
</table>

4. FIRST AID MEASURES

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability
Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature: 2 - 8 °C
Moisture sensitive.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Components</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
Liver damage Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TWA</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td>Skin notation</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>TWA</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td>Skin designation</td>
<td></td>
<td>The value in mg/m3 is approximate.</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td>Potential Occupational Carcinogen See Appendix A 30 minute ceiling value</td>
<td></td>
</tr>
</tbody>
</table>
Personal protective equipment

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).

Hand 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: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatrill® (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 CE 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.

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

Skin and body protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>Appearance</th>
<th></th>
</tr>
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<tbody>
<tr>
<td>Form</td>
<td>liquid</td>
</tr>
<tr>
<td>Colour</td>
<td>no data available</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Safety data</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
</tr>
<tr>
<td>Melting point/freezing point</td>
</tr>
<tr>
<td>Boiling point</td>
</tr>
<tr>
<td>Flash point</td>
</tr>
<tr>
<td>Ignition temperature</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
</tr>
<tr>
<td>Lower explosion limit</td>
</tr>
<tr>
<td>Upper explosion limit</td>
</tr>
</tbody>
</table>
Vapour pressure 23.4647 hPa (17.6000 mmHg) at 37.7 °C (99.9 °F)
Density 0.93 g/mL at 25 °C (77 °F)
Water solubility no data available
Partition coefficient: n-octanol/water no data available
Relative vapour density no data available
Odour no data available
Odour Threshold no data available
Evaporation rate no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
Vapours may form explosive mixture with air.

Conditions to avoid
Heat, flames and sparks.

Materials to avoid
Acids, Oxidizing agents, Alkali metals, Halogens

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity
Oral LD50 no data available
Inhalation LC50 no data available
Dermal LD50 no data available

Other information on acute toxicity
LD50 Intravenous - mouse - 100 mg/kg

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitisation
no data available

Germ cell mutagenicity
no data available

Carcinogenicity
IARC: 2B - Group 2B: Possibly carcinogenic to humans (1,4-Dioxane)
NTP: 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

no data available

**Teratogenicity**

no data available

**Specific target organ toxicity - single exposure (Globally Harmonized System)**

no data available

**Specific target organ toxicity - repeated exposure (Globally Harmonized System)**

no data available

**Aspiration hazard**

May be fatal if swallowed and enters airways.

**Potential health effects**

<table>
<thead>
<tr>
<th>Category</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inhalation</td>
<td>May be harmful if inhaled. Causes respiratory tract irritation.</td>
</tr>
<tr>
<td>Ingestion</td>
<td>May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.</td>
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<tr>
<td>Skin</td>
<td>May be harmful if absorbed through skin. Causes skin irritation.</td>
</tr>
<tr>
<td>Eyes</td>
<td>Causes eye irritation.</td>
</tr>
</tbody>
</table>

**Signs and Symptoms of Exposure**

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.

**Synergistic effects**

no data available

**Additional Information**

RTECS: DA0780000

12. ECOLOGICAL INFORMATION

**Toxicity**

no data available

**Persistence and degradability**

no data available

**Bioaccumulative potential**

no data available

**Mobility in soil**

no data available

**PBT and vPvB assessment**

no data available

**Other adverse effects**

no data available

13. DISPOSAL CONSIDERATIONS

**Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 3295  Class: 3  Packing group: III
Proper shipping name: Hydrocarbons, liquid, n.o.s.
Reportable Quantity (RQ): 10001 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 3295  Class: 3  Packing group: III
Proper shipping name: HYDROCARBONS, LIQUID, N.O.S.
Marine pollutant: No

IATA
UN number: 3295  Class: 3  Packing group: III
Proper shipping name: Hydrocarbons, liquid, n.o.s.

15. REGULATORY INFORMATION

OSHA Hazards
Flammable liquid, Carcinogen, Target Organ Effect, Irritant

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>Revision Date</th>
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</thead>
<tbody>
<tr>
<td>1,4-Dioxane</td>
<td>123-91-1</td>
<td>2007-07-01</td>
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</table>

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

<table>
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Pennsylvania Right To Know Components

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<th>Revision Date</th>
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<td>2007-07-01</td>
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<tr>
<td>1,4-Dioxane</td>
<td>123-91-1</td>
<td>2007-07-01</td>
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New Jersey Right To Know Components

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<td>123-91-1</td>
<td>2007-07-01</td>
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California Prop. 65 Components
WARNING! This product contains a chemical known to the State of California to cause cancer.

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<tbody>
<tr>
<td>1,4-Dioxane</td>
<td>123-91-1</td>
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16. OTHER INFORMATION

Further information
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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.