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

1.1 **Product identifiers**

- **Product name**: 1-Octyne
- **Product Number**: 244465
- **Brand**: Aldrich
- **CAS-No.**: 629-05-0

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 2), H225
- Aspiration hazard (Category 1), H304
- Short-term (acute) aquatic hazard (Category 3), H402

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)**
  - H225: Highly flammable liquid and vapor.
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.

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. Remove contact lenses.

If swallowed

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
Hydrogen bromide gas
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters
In the event of fire, wear self-contained breathing apparatus.

5.4 Further information
Remove container from danger zone and cool with water. 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: 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 protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Change contaminated clothing. Wash hands 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.
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
Contains no substances with occupational exposure limit values.

8.2 Exposure controls
Appropriate engineering controls
Change contaminated clothing. Wash hands 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 30 min
Material tested: Butoject® (KCL 898)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

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

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**SECTION 9: Physical and chemical properties**

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

- **a) Appearance**
  - Form: clear, liquid
  - Color: colorless

- **b) Odor**
  - No data available

- **c) Odor Threshold**
  - No data available

- **d) pH**
  - No data available

- **e) Melting point/freezing point**
  - Melting point/range: -80 °C (-112 °F) - lit.

- **f) Initial boiling point and boiling range**
  - 127 - 128 °C 261 - 262 °F - lit.

- **g) Flash point**
  - 16 °C (61 °F) - closed cup

- **h) Evaporation rate**
  - No data available

- **i) Flammability (solid, gas)**
  - No data available
| j) Upper/lower flammability or explosive limits | Lower explosion limit: 0.8 % (V) |
| k) Vapor pressure | 50.26 hPa at 37.7 °C (99.9 °F) |
| l) Vapor density | No data available |
| m) 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

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### SECTION 10: Stability and reactivity

#### 10.1 Reactivity
Vapors may form explosive mixture with air.

#### 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
- Nitrogen oxides

#### 10.4 Conditions to avoid
Warming.

#### 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**
Acute toxicity estimate Oral - 2,500 mg/kg
(Calculation method)
LD50 Oral - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 420)
Symptoms: Possible damages:, mucosal irritations
Dermal: No data available

**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
Test Type: Hamster
Test system: Liver
Remarks: Unscheduled DNA synthesis

**Carcinogenicity**
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**
No data available

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

RTECS: RI2655000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - 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 Other adverse effects
Discharge into the environment must be avoided.

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: II
Proper shipping name: Hydrocarbons, liquid, n.o.s.
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

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

IATA
UN number: 3295  Class: 3  Packing group: II
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
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
No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components
<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-octyne</td>
<td>629-05-0</td>
<td></td>
</tr>
<tr>
<td>1-Bromohexane</td>
<td>111-25-1</td>
<td></td>
</tr>
</tbody>
</table>

New Jersey Right To Know Components
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</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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