SAFETY DATA SHEET
according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 05/22/2017  Version 2.0

SECTION 1. Identification

Product identifier

<table>
<thead>
<tr>
<th>Product number</th>
<th>820735</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product name</td>
<td>1-Iodohexadecane for synthesis</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>544-77-4</td>
</tr>
</tbody>
</table>

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

- Identified uses: Chemical for synthesis

Details of the supplier of the safety data sheet

- Company: EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
- MilliporeSigma is a business of Merck KGaA, Darmstadt, Germany.

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

SECTION 2. Hazards identification

GHS Classification

- Flammable liquid, Category 4, H227

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

GHS-Labeling

- Signal Word: Warning

Precautionary Statements

- P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P403 + P235 Store in a well-ventilated place. Keep cool.
- P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

- None known.
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Product number 820735
Product name 1-Iodohexadecane for synthesis

SECTION 3. Composition/information on ingredients

Formula \( \text{CH}_3(\text{CH}_2)_{15}\text{I} \quad \text{C}_{16}\text{H}_{33}\text{I} \) (Hill)
Molar mass 352.34 g/mol

Hazardous ingredients

Chemical name (Concentration)
CAS-No.
Iodohexadecane \( (\geq 90\% - \leq 100\%) \)
544-77-4

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation
After inhalation: fresh air.

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

Eye contact
After eye contact: rinse out with plenty of water. Remove contact lenses.

Ingestion
After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

The following applies to aliphatic halogenated hydrocarbons in general: systemic effect: narcosis, cardiovascular disorders. Toxic effect on liver, kidneys.

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture

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 vapors possible in the event of fire. Fire may cause evolution of:
hydrogen iodide

Advice for firefighters

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.

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

Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Avoid inhalation of dusts. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment 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

Precautions for safe handling
Observe label precautions.

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

Conditions for safe storage, including any incompatibilities
Tightly closed. Dry.
Store below +30°C (+86°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)
Contains no substances with occupational exposure limit values.

Engineering measures
Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.
Individual protection measures
Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures
Change contaminated clothing. Wash hands after working with substance.

Eye/face protection
Safety glasses

Hand protection
full contact:
- Glove material: Nitrile rubber
- Glove thickness: 0.11 mm
- Break through time: > 480 min

splash contact:
- Glove material: Nitrile rubber
- Glove thickness: 0.11 mm
- Break through time: > 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).
The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.
This recommendation applies only to the product stated in the safety data sheet and supplied by us as well as to the purpose specified by us. 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).

Other protective equipment:
Flame retardant antistatic protective clothing.

Respiratory protection
required when dusts are generated.
Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are performed according to the instructions of the producer. These measures have to be properly documented.

SECTION 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Physical state</th>
<th>solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Color</td>
<td>colorless</td>
</tr>
<tr>
<td>Odor</td>
<td>No strong odor known.</td>
</tr>
<tr>
<td>Odor Threshold</td>
<td>No information available.</td>
</tr>
<tr>
<td>pH</td>
<td>No information available.</td>
</tr>
</tbody>
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<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting point</td>
<td>68 - 73 °F (20 - 23 °C)</td>
</tr>
<tr>
<td></td>
<td>at 1,013 hPa</td>
</tr>
<tr>
<td>Boiling point/boiling range</td>
<td>414 °F (212 °C)</td>
</tr>
<tr>
<td></td>
<td>at 20 hPa</td>
</tr>
<tr>
<td>Flash point</td>
<td>161.6 - 162.5 °F (72.0 - 72.5 °C)</td>
</tr>
<tr>
<td></td>
<td>at 1,013 hPa</td>
</tr>
<tr>
<td>Method</td>
<td>c.c.</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No information available.</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No information available.</td>
</tr>
<tr>
<td>Lower explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Upper explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>No information available.</td>
</tr>
<tr>
<td>Relative vapor density</td>
<td>No information available.</td>
</tr>
<tr>
<td>Density</td>
<td>1.12 g/cm³</td>
</tr>
<tr>
<td></td>
<td>at 68 °F (20 °C)</td>
</tr>
<tr>
<td>Relative density</td>
<td>No information available.</td>
</tr>
<tr>
<td>Water solubility</td>
<td>0.02 µg/l</td>
</tr>
<tr>
<td></td>
<td>at 68 °F (20 °C)</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>log Pow: 8.96 (calculated)</td>
</tr>
<tr>
<td></td>
<td>(Lit.) A remarkable bioaccumulation potential is expected (log Po/w &gt;3).</td>
</tr>
<tr>
<td>Autoignition temperature</td>
<td>No information available.</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No information available.</td>
</tr>
<tr>
<td>Viscosity, dynamic</td>
<td>No information available.</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Not classified as explosive.</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>none</td>
</tr>
</tbody>
</table>

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**
- Sensitivity to light

**Possibility of hazardous reactions**
- Violent reactions possible with:
  - Strong oxidizing agents

**Conditions to avoid**
- Strong heating.

**Incompatible materials**
- no information available

**Hazardous decomposition products**
- in the event of fire: See section 5.

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**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*
- Eye contact, Skin contact

*Specific target organ systemic toxicity - single exposure*
- The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ systemic toxicity - repeated exposure*
- The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*
- Regarding the available data the classification criteria are not fulfilled.

**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.

- **OSHA**
  - No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

- **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.

- **ACGIH**
  - No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
Further information
Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.
The following applies to aliphatic halogenated hydrocarbons in general: systemic effect: narcosis, cardiovascular disorders. Toxic effect on liver, kidneys.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity
Toxicity to fish
LC50 Oncorhynchus mykiss (rainbow trout): > 30 mg/l; 96 h The product has low solubility in the test medium. An aqueous dispersion was tested.
Toxicity to daphnia and other aquatic invertebrates
EC50 Daphnia pulex (Water flea): 0.219 mg/l; 48 h The product has low solubility in the test medium. An aqueous dispersion was tested.

Persistence and degradability
No information available.

Bioaccumulative potential
Partition coefficient: n-octanol/water
log Pow: 8.96 (calculated)
(Lit.) A remarkable bioaccumulation potential is expected (log Po/w >3).

Mobility in soil
No information available.

Additional ecological information
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations
The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)
UN number UN 3082
Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-IODO HEXADECANE)
Class 9
Packing group III
Environmentally hazardous --

Air transport (IATA)
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Product number  820735
Product name  1-Iodohexadecane for synthesis

UN number  UN 3082
Proper shipping name  ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-IODO HEXADECANE)
Class  9
Packing group  III
Environmentally hazardous  --
Special precautions for user  no

Sea transport (IMDG)
UN number  UN 3082
Proper shipping name  ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-IODO HEXADECANE)
Class  9
Packing group  III
Environmentally hazardous  --
Special precautions for user  yes
EmS  F-A  S-F

SECTION 15. Regulatory information
United States of America

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.

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

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

DEA List I
Not listed

DEA List II
Not listed

US State Regulations

Massachusetts Right To Know
Remarks
No components are subject to the Massachusetts Right to Know Act.
California Prop 65 Components
This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status
TSCA: All components of the product are listed in the TSCA-inventory.

DSL: This product contains one or several components listed in the Canadian NDSL.

SECTION 16. Other information

Training advice
Provide adequate information, instruction and training for operators.

Labeling
Hazard pictograms

Signal Word
Warning

Hazard Statements
H227 Combustible liquid.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements
Prevention
P273 Avoid release to the environment.

Full text of H-Statements referred to under sections 2 and 3.
H227 Combustible liquid.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Revision Date 05/22/2017

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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