



# MATERIAL SAFETY DATA SHEET

according to the Global Harmonized System

Date of issue: 02/04/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number 804786  
Product name 1-Iodobutane for synthesis

### 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 | SDS Phone Support: +1-978-715-1335 |  
General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to  
4:00 PM Eastern Time (GMT-5)  
  
e-mail: mm\_sds@merckgroup.com

Emergency telephone 613-996-6666 CANUTEC (Canada)  
+1-703-527-3887 CHEMTREC (International)  
24 Hours/day; 7 Days/week

## SECTION 2. Hazards identification

### GHS Classification

Flammable liquid, Category 3, H226  
Acute toxicity, Category 3, Inhalation, H331  
For the full text of the H-Statements mentioned in this Section, see Section 16.

### GHS-Labeling

#### Hazard pictograms



Signal Word  
Danger

#### Hazard Statements

H226 Flammable liquid and vapor.  
H331 Toxic if inhaled.

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*Precautionary Statements*

P210 Keep away from heat.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

**Other hazards**

None known.

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**SECTION 3. Composition/information on ingredients**

Formula	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> I	C <sub>4</sub> H <sub>9</sub> I (Hill)
CAS-No.	542-69-8	
Molar mass	184.02 g/mol	

**Hazardous ingredients**

*Chemical Name (Concentration)*

CAS-No.

1-iodobutane (>= 90 % - <= 100 % )

542-69-8

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**SECTION 4. First aid measures**

**Description of first-aid measures**

*General advice*

First aider needs to protect himself.

*Inhalation*

After inhalation: fresh air. If breathing stops: immediately apply artificial respiration, if necessary oxygen. Immediately call in physician.

*Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

*Eye contact*

After eye contact: rinse out with plenty of water.

*Ingestion*

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

Never give anything by mouth to an unconscious person.

**Most important symptoms and effects, both acute and delayed**

irritant effects, Cough, Shortness of breath, Diarrhea, Gastrointestinal discomfort, Nausea, Vomiting, Headache

**Indication of any immediate medical attention and special treatment needed**

No information available.

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**SECTION 5. Fire-fighting measures**

**Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, 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 material

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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*

Suppress (knock down) gases/vapors/mists with a water spray jet. Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6. Accidental release measures**

**Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

**Environmental precautions**

Do not empty into drains. Risk of explosion.

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

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**SECTION 7. Handling and storage**

**Precautions for safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

Observe label precautions.

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*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**

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

Store at +15°C to +25°C (+59°F to +77°F).

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**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. Application of skin- protective barrier cream recommended. Wash hands after working with substance. Work under hood. Do not inhale substance/mixture.

*Eye/face protection*

Safety glasses

*Hand protection*

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

*Other protective equipment:*

Flame retardant antistatic protective clothing

*Respiratory protection*

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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**SECTION 9. Physical and chemical properties**

Physical state	liquid
Color	colorless
Odor	ether-like
Odor Threshold	No information available.

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pH	No information available.
Melting point	-103 °C
Boiling point/boiling range	266 °F (130 °C) at 1,013 hPa
Flash point	91 °F (33 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	18.5 hPa at 77 °F (25 °C)
Relative vapor density	6.35
Relative density	1.62 g/cm <sup>3</sup> at 68 °F (20 °C)
Water solubility	0.2 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 3.06 (calculated) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	Distillable in an undecomposed state at normal pressure.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.

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**SECTION 10. Stability and reactivity**

**Reactivity**

Vapor/air-mixtures are explosive at intense warming.

**Chemical stability**

Sensitivity to light

Sensitive to air.

**Possibility of hazardous reactions**

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Violent reactions possible with:  
Strong oxidizing agents, Bases, Alkali metals

**Conditions to avoid**

Heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**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*

Inhalation, Eye contact, Skin contact

*Acute oral toxicity*

Symptoms: Gastrointestinal discomfort, Nausea, Vomiting, Diarrhea

*Acute inhalation toxicity*

LC50 rat: 6.1 mg/l; 4 h (RTECS)

Symptoms: mucosal irritations, Cough, Shortness of breath

absorption

*Sensitization*

Sensitization possible in predisposed persons.

*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

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carcinogen by ACGIH.

**Further information**

After absorption:  
Headache  
Further data:  
Other dangerous properties can not be excluded.  
This substance should be handled with particular care.

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**SECTION 12. Ecological information**

**Ecotoxicity**

No information available.

**Persistence and degradability**

No information available.

**Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 3.06

(calculated)

(Lit.) Bioaccumulation is not expected (log Pow <1).

**Mobility in soil**

No information available.

**Other adverse effects**

*Additional ecological information*

Discharge into the environment must be avoided.

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**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.

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**SECTION 14. Transport information**

**Land transport (DOT)**

UN number	UN 1993
Proper shipping name	FLAMMABLE LIQUID, N.O.S. (1-iodobutane)
Class	3
Packing group	III
Environmentally hazardous	--

**Air transport (IATA)**

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**UN number** UN 1993  
**Proper shipping name** FLAMMABLE LIQUID, N.O.S. (1-IODOBUTANE)  
**Class** 3  
**Packing group** III  
**Environmentally hazardous** --  
**Special precautions for user** no

**Sea transport (IMDG)**

**UN number** UN 1993  
**Proper shipping name** FLAMMABLE LIQUID, N.O.S. (1-IODOBUTANE)  
**Class** 3  
**Packing group** III  
**Environmentally hazardous** --  
**Special precautions for user** yes  
**EmS** F-E S-E

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**SECTION 15. Regulatory information**

**United States of America**

**Canada**

**WHMIS Classification**

B2 Flammable Liquid  
D1A Very Toxic Material Causing Immediate and Serious Toxic Effects

Flammable Liquid, Highly toxic by inhalation

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

**Notification status**

TSCA: On TSCA Inventory

DSL: All components of this product are on the Canadian DSL.

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**SECTION 16. Other information**

**Training advice**

Provide adequate information, instruction and training for operators.

**Full text of H-Statements referred to under sections 2 and 3.**

H226 Flammable liquid and vapor.  
H331 Toxic if inhaled.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

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Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

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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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