



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

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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.

SECTION 3. Composition/information on ingredients

Formula	CH ₃ (CH ₂) ₃ I	C ₄ H ₉ 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

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 (CO₂), 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.

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. Chemisorb®). Dispose of properly. Clean up affected area.

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).

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.

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 ³ 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.

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.

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.

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.

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 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

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.

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.

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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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