



MATERIAL SAFETY DATA SHEET

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

Revision Date 08/23/2013

Version 1.1

SECTION 1. Identification

Product identifier

Product number	801556
Product name	Isobutyraldehyde for synthesis

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

Identified uses	Chemical for synthesis
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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: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 2, H225

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

GHS-Labeling

Hazard pictograms



Signal Word

Danger

Hazard Statements

H225 Highly flammable liquid and vapor.

Precautionary Statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P233 Keep container tightly closed.

P403 + P235 Store in a well-ventilated place. Keep cool.

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OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	(CH ₃) ₂ CHCHO	C ₄ H ₈ O (Hill)
CAS-No.	78-84-2	
Molar mass	72.11 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

isobutyraldehyde (>= 90 % - <= 100 %)

78-84-2

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

Dermatitis

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture

Combustible.

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

Advice for firefighters

Special protective equipment for fire-fighters

In the event of fire, wear self-contained breathing apparatus.

Further information

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 substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. 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 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

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

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place. Protected from light.

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.

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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.

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	stinging
Odor Threshold	No information available.
pH	No information available.
Melting point	-65 °C
Boiling point/boiling range	145 - 148.1 °F (63 - 64.5 °C) at 1,013 mbar
Flash point	-4 °F (-20 °C) Method: DIN 51755 Part 1
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1.6 %(V)
Upper explosion limit	11.0 %(V)

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Vapor pressure	189 hPa at 68 °F (20 °C)
	640 hPa at 122 °F (50 °C)
Relative vapor density	2.48
Relative density	0.79 g/cm ³ at 68 °F (20 °C) Method: DIN 51757
Water solubility	75 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 0.77 (25 °C) OECD Test Guideline 107 Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0.5 mPa.s at 68 °F (20 °C)
Explosive properties	Not classified as explosive.
Ignition temperature	329 °F (165 °C) Method: DIN 51794
Saturated vapor concentration	452 g/m ³

SECTION 10. Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

Sensitivity to light

Sensitive to air.

Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapors with:

Strong oxidizing agents, Strong acids, strong reducing agents

Exothermic reaction with:

alkaline substances, Strong bases

Conditions to avoid

Warming.

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

Incompatible materials

no information available

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Acute oral toxicity

LD50 rat: > 3,000 mg/kg (External MSDS)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

Acute inhalation toxicity

Symptoms: Inhalation may lead to the formation of oedemas in the respiratory tract., Symptoms may be delayed.

Acute dermal toxicity

LD50 rabbit: > 5,000 mg/kg
(External MSDS)

Skin irritation

rabbit

Result: No irritation

OECD Test Guideline 404

After long-term exposure to the chemical:

Dermatitis

Eye irritation

rabbit

Result: No eye irritation

OECD Test Guideline 405

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

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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

Further hazardous properties cannot be excluded but unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 23 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 277 mg/l; 48 h (Lit.)

Toxicity to algae

IC50 Desmodesmus subspicatus (green algae): 84 mg/l; 72 h (IUCLID)

Toxicity to bacteria

EC50 Pseudomonas putida: 468 mg/l; 17 h (IUCLID)

Persistence and degradability

Biodegradability

> 95 %; 5 d

OECD Test Guideline 302B

Readily eliminated from water

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0.77 (25 °C)

OECD Test Guideline 107

Bioaccumulation is not expected (log Pow <1).

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.

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SECTION 14. Transport information

Land transport (DOT)

UN number UN 2045
Proper shipping name ISOBUTYRALDEHYDE
Class 3
Packing group II
Environmentally hazardous --

Air transport (IATA)

UN number UN 2045
Proper shipping name ISOBUTYRALDEHYDE
Class 3
Packing group II
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 2045
Proper shipping name ISOBUTYRALDEHYDE
Class 3
Packing group II
Environmentally hazardous --
Special precautions for user yes
EmS F-E S-D

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Flammable Liquid

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard

SARA 313

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

Ingredients

isobutyraldehyde 78-84-2

SARA 302

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

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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.

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

Ingredients
isobutyraldehyde

Pennsylvania Right To Know

Ingredients
isobutyraldehyde

New Jersey Right To Know

Ingredients
isobutyraldehyde

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: 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.

H225 Highly flammable liquid and vapor.

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.

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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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