

• SAFETY DATA SHEET

Version 6.7
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isobutyraldehyde
Product Number : 320358
Brand : Aldrich
CAS-No. : 78-84-2

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

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 2

Eye irritation : Category 2A

Short-term (acute) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :  

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P264 Wash skin thoroughly after handling.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

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

Disposal:

P501 Dispose of contents/ container to an approved

waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 78-84-2

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
isobutyraldehyde	78-84-2*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this 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. Call in ophthalmologist. Remove contact lenses.

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

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Carbon dioxide (CO2)
Foam
Dry powder

Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Pay attention to flashback.
	Vapours 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.
Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, 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.
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Advice for emergency responders:
For personal protection see section 8.

Environmental precautions : Do not let product enter 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

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

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
isobutyraldehyde	78-84-2	TWA	25 ppm	US WEEL

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter type AX

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : butyl-rubber
Break through time : 60 min
Glove thickness : 0.7 mm
Protective index : Splash contact
Manufacturer : Butoject® (KCL 898)

Remarks : 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection

: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

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

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : colourless

Odor : unpleasant

Odor Threshold : No data available
pH : No data available

Melting point/ range : -85 °F / -65 °C

	Method: lit.
Boiling point/boiling range	: 145 °F / 63 °C Method: lit.
Flash point	: -11 °F / -24 °C (1,013 hPa) Method: DIN 51755 Part 1, closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: 356 °F / 180 °C 1,013.25 hPa Method: ASTM E-659
Upper explosion limit / Upper flammability limit	: 11.0 %(V)
Lower explosion limit / Lower flammability limit	: 1.6 %(V)
Vapor pressure	: 88 hPa (39.9 °F / 4.4 °C) 189 hPa (68 °F / 20 °C) 640 hPa (122 °F / 50 °C)
Relative vapour density	: 2.49 (Air = 1.0)
Relative density	: No data available
Density	: 0.79 g/cm3 (77 °F / 25 °C) Method: lit.
Solubility(ies)	
Water solubility	: 60 g/l (77 °F / 25 °C) Method: OECD Test Guideline 105
Partition coefficient: n-octanol/water	: log Pow: 0.77 (77 °F / 25 °C) Method: OECD Test Guideline 107 Bioaccumulation is not expected.
Autoignition temperature	: 374 °F / 190 °C
Decomposition	: No data available

temperature

Viscosity

Viscosity, dynamic : 0.43 mPa.s (68 °F / 20 °C)

Viscosity, kinematic : No data available

Flow time : No data available

Explosive properties : No data available

Oxidizing properties : none

Molecular weight : 72.11 g/mol

Particle characteristics

Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : Vapours may form explosive mixture with air.

Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : Risk of ignition or formation of inflammable gases or vapours with:
Strong oxidizing agents
Strong acids
strong reducing agents
Exothermic reaction with:
alkaline substances
Strong bases

Conditions to avoid : Warming.

Incompatible materials : No data available

Hazardous decomposition : In the event of fire: see section 5 products

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 3,730 mg/kg

(OECD Test Guideline 401)

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

LC50 Inhalation - Rat - male - 4 h - > 23.6 mg/l - vapour

(OECD Test Guideline 403)

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

LD50 Dermal - Rabbit - male - 5,583 mg/kg

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Remarks: After long-term exposure to the chemical:

Dermatitis

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation. - 24 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component 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 component 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

No data available

11.2 Additional Information

RTECS: NQ4025000

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

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

isobutyraldehyde:

Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 23 mg/l
End point: mortality
Exposure time: 96 h
Test Type: static test
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 277 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: static test
Method: Regulation (EC) No. 440/2008, Annex, C.2
Remarks: (above the solubility limit in the test medium)

Toxicity to algae/aquatic plants : ErC50 (Desmodesmus subspicatus (green algae)): 83.7 mg/l
Exposure time: 72 h
Test Type: static test
Method: DIN 38412
Remarks: (above the solubility limit in the test medium)

Toxicity to microorganisms : NOEC (activated sludge): 100 mg/l
Exposure time: 14 Days
Test Type: static test
Remarks: (ECHA)

Ecotoxicology Assessment

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

isobutyraldehyde:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Readily biodegradable.
Biodegradation: 80 - 90 %
Exposure time: 14 d
Method: OECD Test Guideline 301C

Bioaccumulative potential

Components:

isobutyraldehyde:

Partition coefficient: n-octanol/water : log Pow: 0.77 (77 °F / 25 °C)
Method: OECD Test Guideline 107
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

isobutyraldehyde:

Additional ecological information : Discharge into the environment must be avoided.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 2045
Proper shipping name : Isobutyl aldehyde
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 364
Packing instruction (passenger aircraft) : 353

IMDG-Code

UN number : UN 2045
Proper shipping name : ISOBUTYL ALDEHYDE

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-D

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Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2045
Proper shipping name : Isobutyl aldehyde

Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
ERG Code : 130
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard

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

isobutyraldehyde 78-84-2 >= 90 - <= 100 %
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US State Regulations

Massachusetts Right To Know

isobutyraldehyde 78-84-2

Pennsylvania Right To Know

isobutyraldehyde 78-84-2

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

US WEEL : USA. Workplace Environmental Exposure Levels (WEEL)

US WEEL / TWA : 8-hr TWA

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA -

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Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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