

1. Identification

Product identifier	Isobutyraldehyde	
Other means of identification		
Catalog number	1347880	
Chemical name	Propanal, 2-methyl-	
Synonym(s)	Isobutanal	
Recommended use	Specified quality tests and assay use only.	
Recommended restrictions	Not for use as a drug. Not for administration to humans or animals.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	U. S. Pharmacopeia	
Address	12601 Twinbrook Parkway Rockville MD 20852-1790 United States	
Telephone	RS Technical Services	301-816-8129
Website	www.usp.org	
E-mail	RSTECH@usp.org	
Emergency phone number	CHEMTREC within US & Canada	1-800-424-9300
	CHEMTREC outside US & Canada	+1 703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 2
Health hazards	Acute toxicity, oral	Category 4
	Skin corrosion/irritation	Category 2
	Serious eye damage/eye irritation	Category 2A
	Specific target organ toxicity, single exposure	Category 3 respiratory tract irritation
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		



Signal word	Danger
Hazard statement	Highly flammable liquid and vapor. Harmful if swallowed. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Use only outdoors or in a well-ventilated area. Keep container tightly closed. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Avoid breathing mist or vapor. Wash thoroughly after handling. Wear protective gloves/eye protection/face protection.
Response	If swallowed: Call a poison center/doctor if you feel unwell. Rinse mouth. If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. If skin irritation occurs: Get medical advice/attention. Wash contaminated clothing before reuse. If inhaled: Remove person to fresh air and keep comfortable for breathing. Call a poison center/doctor if you feel unwell. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention. In case of fire: Use appropriate media for extinction.
Storage	Store in a well-ventilated place. Keep container tightly closed. Store locked up. Keep cool.
Disposal	Dispose of contents/container in accordance with local/regional/national/international regulations.

Hazard(s) not otherwise classified (HNOC) Static accumulating flammable liquids

Other hazards which do not result in classification None known.

3. Composition/information on ingredients

Substance

Chemical name	Common name and synonyms	CAS number	%
Isobutyraldehyde	Isobutanol	78-84-2	100

4. First-aid measures

Inhalation	Move to fresh air. Oxygen or artificial respiration if needed. Do not use mouth-to-mouth method if victim inhaled the substance. Call a physician if symptoms develop or persist.
Skin contact	Rinse skin with water/shower. Get medical attention if irritation develops and persists.
Eye contact	Immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth thoroughly. Do not induce vomiting without advice from poison control center. Do not use mouth-to-mouth method if victim ingested the substance. IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
Most important symptoms/effects, acute and delayed	Irritant effects.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically.
General information	Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO ₂).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	This product is a poor conductor of electricity and can become electrostatically charged. If sufficient charge is accumulated, ignition of flammable mixtures can occur. To reduce potential for static discharge, use proper bonding and grounding procedures. This liquid may accumulate static electricity when filling properly grounded containers. Static electricity accumulation may be significantly increased by the presence of small quantities of water or other contaminants. By heating and fire, harmful vapors/gases may be formed. Material will float and may ignite on surface of water.
Special protective equipment and precautions for firefighters	Wear suitable protective equipment.
Fire-fighting equipment/instructions	As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.
Specific methods	Cool containers exposed to flames with water until well after the fire is out.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Keep unnecessary personnel away. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. Avoid inhalation of vapors. Wear appropriate personal protective equipment.
Methods and materials for containment and cleaning up	ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Absorb spillage with non-combustible, absorbent material. For waste disposal, see section 13 of the SDS. Wash spill site.

7. Handling and storage

Precautions for safe handling	Keep away from open flames, hot surfaces and sources of ignition. As a general rule, when handling USP Reference Standards, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Use of a designated area is recommended for handling of potent materials.
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Conditions for safe storage, including any incompatibilities

Eliminate sources of ignition. Store in tight container as defined in the USP-NF. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits

US. Workplace Environmental Exposure Level (WEEL) Guides

Material	Type	Value
Isobutyraldehyde (CAS 78-84-2)	TWA	25 ppm

Biological limit values

No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls

Airborne exposure should be controlled primarily by engineering controls such as general dilution ventilation, local exhaust ventilation, or process enclosure. Local exhaust ventilation is generally preferred to general exhaust because it can control the contaminant at its source, preventing dispersion into the work area. An industrial hygiene survey involving air monitoring may be used to determine the effectiveness of engineering controls. Effectiveness of engineering controls intended for use with highly potent materials should be assessed by use of nontoxic surrogate materials. Local exhaust ventilation such as a laboratory fume hood or other vented enclosure is recommended, particularly for aerosol-generating procedures.

Individual protection measures, such as personal protective equipment

Eye/face protection

Safety glasses with sideshields are recommended. Face shields or goggles may be required if splash potential exists or if corrosive materials are present. Approved eye protection (e.g., bearing the ANSI Z87 or CSA stamp) is preferred. Maintain eyewash facilities in the work area.

Skin protection

Hand protection

Chemically compatible gloves. For handling solutions, ensure that the glove material is protective against the solvent being used. Use handling practices that minimize direct hand contact. Employees who are sensitive to natural rubber (latex) should use nitrile or other synthetic nonlatex gloves. Use of powdered latex gloves should be avoided due to the risk of latex allergy.

Other

For handling of laboratory scale quantities, a cloth lab coat is recommended. Where significant quantities are handled, work clothing may be necessary to prevent take-home contamination.

Respiratory protection

Where respirators are deemed necessary to reduce or control occupational exposures, use NIOSH-approved respiratory protection and have an effective respirator program in place (applicable U.S. regulation OSHA 29 CFR 1910.134).

General hygiene considerations

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Clear, colorless liquid.

Physical state

Liquid.

Form

Liquid.

Odor

Pungent odor.

Odor threshold

0.14 - 0.3 ppm
> 2 ppb

pH

Not available.

Melting point/freezing point

-84.1 - -86.8 °F (-64.5 - -66 °C)

Initial boiling point and boiling range

145.4 - 147.38 °F (63 - 64.1 °C)

Flash point

-40.0 °F (-40.0 °C) Closed Cup
-11.0 - 19.9 °F (-23.9 - -6.7 °C) Open Cup

Evaporation rate

Not available.

Flammability (solid, gas)

Not applicable.

Upper/lower flammability or explosive limits

Flammability limit - lower (%)

1.6 %

Flammability limit - upper (%)

10.6 %

Explosive limit - lower (%)

Not available.

Explosive limit - upper (%)

Not available.

Vapor pressure

22.9 - 23.06 kPa at 25 °C
173 mm Hg at 25 °C

Vapor density

2.48 - 2.5

Relative density

Not available.

Solubility in water	Soluble.
Partition coefficient (n-octanol/water)	0.77 - 1.2
Auto-ignition temperature	374 - 384.98 °F (190 - 196.1 °C)
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Dynamic viscosity	0.45 - 0.54 mPa.s
Dynamic viscosity temperature	82.76 °F (28.2 °C)
Molecular formula	C4H8O
Molecular weight	72.11
Percent volatile	100 %
Solubility (other)	Miscible with ethanol, with ether, with carbon disulfide, with acetone, with benzene, with toluene, and with chloroform; slightly soluble in carbon tetrachloride.
Specific gravity	0.79 - 0.79 at 20 °C
VOC (Weight %)	100 %

10. Stability and reactivity

Reactivity	Not available.
Chemical stability	Risk of ignition.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Ignition sources. Avoid temperatures exceeding the flash point.
Incompatible materials	Strong oxidizing agents. Strong reducing agents. Strong bases.
Hazardous decomposition products	Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions.

11. Toxicological information

Information on likely routes of exposure

Ingestion	Harmful if swallowed.
Inhalation	May cause irritation to the respiratory system.
Skin contact	Causes skin irritation.
Eye contact	Causes serious eye irritation.
Symptoms related to the physical, chemical, and toxicological characteristics	Nausea. Vomiting. Diarrhea. Sore throat. Cough. Sweet, burning taste. Vision loss. Abdominal pain.
Delayed and immediate effects of exposure	Shock. Pulmonary edema.
Acute toxicity	Harmful if swallowed.

Product	Species	Test Results
Isobutyraldehyde (CAS 78-84-2)		
<u>Acute</u>		
Dermal		
LD50	Rabbit	5630 mg/kg
Inhalation		
LC50	Mouse	39.5 mg/l, 2 Hours
Oral		
LD50	Rat	960 mg/kg
Skin corrosion/irritation	Causes skin irritation.	
Serious eye damage/eye irritation	Causes serious eye irritation.	

Local effects

Irritation/Corrosivity test (100 mg)

Result: Irritant.

Species: Rabbit

Organ: Eyes.

Test Duration: 24 hr

Severity: Moderate.

Irritation/Corrosivity test (500 mg)

Result: Irritant.

Species: Rabbit

Organ: Skin.

Test Duration: 24 hr

Severity: Severe.

Open Draize test (20 mg)

Result: Irritant.

Species: Rabbit

Organ: Eyes.

Severity: Severe.

Open Draize test (397 mg)

Result: Irritant.

Species: Rabbit

Organ: Skin.

Severity: Mild.

Respiratory or skin sensitization

Respiratory sensitization Based on available data, the classification criteria are not met.

Skin sensitization Based on available data, the classification criteria are not met.

Skin sensitization

30 % Sensitization test, (material applied to shaved and abraded ears with and without adjuvant)

Result: Non-sensitizing.

Species: Mouse

Organ: Skin.

Test Duration: 5 days

Germ cell mutagenicity

Classification not possible.

Results for genotoxicity and mutagenicity studies were mixed.

Carcinogenicity

Based on available data, the classification criteria are not met.

This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.

Did not cause cancer in long-term animal studies.

Reproductive toxicity

Based on available data, the classification criteria are not met. No fertility impairing effects were seen in animal studies. No indications of developmental toxicity or teratogenic effects were seen in animal studies.

Specific target organ toxicity - single exposure

Respiratory tract irritation.

Specific target organ toxicity - repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

12. Ecological information

Ecotoxicity

No ecotoxicity data noted for the ingredient(s).

Persistence and degradability

No data is available on the degradability of this product.

Bioaccumulative potential

Not available.

Mobility in soil

Not available.

Other adverse effects

Not available.

13. Disposal considerations

Disposal instructions

Dispose in accordance with all applicable regulations.

Local disposal regulations

Not available.

Hazardous waste code

D001: Waste Flammable material with a flash point <140 F

Waste from residues / unused products

Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Empty containers should be taken to an approved waste handling site for recycling or disposal. Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information

DOT

UN number	UN2045
UN proper shipping name	Isobutyraldehyde or Isobutyl aldehyde
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	II
Packaging exceptions	150
Packaging non bulk	202
Packaging bulk	242

IATA

UN number	UN2045
UN proper shipping name	Isobutyraldehyde
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	II
Other information	
Passenger and cargo aircraft	Allowed.
Cargo aircraft only	Allowed.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

DOT



IATA



15. Regulatory information

US federal regulations All components are on the U.S. EPA TSCA Inventory List.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories	Immediate Hazard - Yes
	Delayed Hazard - No
	Fire Hazard - Yes
	Pressure Hazard - No
	Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

SARA 313 (TRI reporting)

Chemical name	CAS number	% by wt.
Isobutyraldehyde	78-84-2	100

Other federal regulations

Safe Drinking Water Act (SDWA) Not regulated.

Food and Drug Administration (FDA) Not regulated.

US state regulations

This product does not contain a chemical known to the State of California to cause cancer, birth defects or other reproductive harm.

US. California Proposition 65

Not Listed.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 05-17-2012

Revision date 09-08-2015

Version # 03

Further information Not available.

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Revision Information This document has undergone significant changes and should be reviewed in its entirety.