

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : Isobutanol

Product Number : W217905
Brand : Aldrich
Index-No. : 603-108-00-1

CAS-No. : 78-83-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USATelephone : +1 800-325-5832
Fax : +1 800-325-5052**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)

H226

Flammable liquid and vapour.

H315

Causes skin irritation.

H318

Causes serious eye damage.

H335

May cause respiratory irritation.

H336

May cause drowsiness or dizziness.

Precautionary statement(s)

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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Isobutanol
2-Methyl-1-propanol
Isobutyl alcohol

Formula : C₄H₁₀O
Molecular weight : 74.12 g/mol
CAS-No. : 78-83-1
EC-No. : 201-148-0
Index-No. : 603-108-00-1

Hazardous components

Component	Classification	Concentration
iso-Butanol		
	Flam. Liq. 3; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H315, H318, H335, H336	<= 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION**8.1 Control parameters**

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
iso-Butanol	78-83-1	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Eye irritation Skin irritation		
		TWA	50.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Eye irritation Skin irritation		
		TWA	100.000000 ppm 300.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	50.000000 ppm 150.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	50 ppm 150 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 300 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	50 ppm 150 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	50 ppm 150 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an

industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: liquid
Colour: colourless, clear |
| b) Odour | alcohol-like |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -108 °C (-162 °F) - lit. |
| f) Initial boiling point and boiling range | 108 °C (226 °F) - lit. |
| g) Flash point | 28 °C (82 °F) - closed cup |
| h) Evaporation rate | 0.6 |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 10.6 %(V)
Lower explosion limit: 1.7 %(V) |
| k) Vapour pressure | 8 hPa (6 mmHg) at 20 °C (68 °F) |
| l) Vapour density | 2.55 |
| m) Relative density | 0.803 g/cm ³ at 25 °C (77 °F) |
| n) Water solubility | 70 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - completely miscible |
| o) Partition coefficient: n-octanol/water | log Pow: 1 at 25 °C (77 °F) |
| p) Auto-ignition temperature | 427 °C (801 °F) |
| q) Decomposition temperature | No data available |
| r) Viscosity | 4.00 mm ² /s at 20 °C (68 °F) - |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

- | | |
|-------------------------|----------------------------|
| Surface tension | 69.7 mN/m at 20 °C (68 °F) |
| Relative vapour density | 2.55 |

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents, Acid chlorides, Acid anhydrides Strong oxidizing agents, Acid chlorides, Acid anhydrides

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 3,350 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 24.6 mg/l

LD50 Dermal - Rabbit - female - 2,460 mg/kg
(OECD Test Guideline 402)

LD50 Intraperitoneal - Rat - 720 mg/kg

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes. - 24 h
(OECD Test Guideline 405)

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

Hamster

fibroblast

Result: negative

OECD Test Guideline 474

Mouse - male and female

Result: negative

Carcinogenicity

Carcinogenicity - Rat - Oral

Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Skin and Appendages: Other: Tumors. Leukaemia

Carcinogenicity - Rat - Subcutaneous

Tumorigenic: Carcinogenic by RTECS criteria. Gastrointestinal: Tumors. Liver: Tumors.

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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

Reproductive toxicity - Rat - male and female - inhalation (vapour)

No significant adverse effects were reported

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory Tract

May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity Rat - male and female - inhalation (vapour) - NOAEL : ≥ 7.5 mg/l - OECD Test Guideline 408

RTECS: NP9625000

Cough, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,430 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia pulex (Water flea) - 1,100 mg/l - 48 h

Toxicity to algae static test EC50 - Pseudokirchneriella subcapitata - 1,799 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria Growth inhibition IC50 - Sludge Treatment - $> 1,000$ mg/l - 16 h

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 70 - 80 % - Readily biodegradable (OECD Test Guideline 301D)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN number: 1212 Class: 3 Packing group: III
Proper shipping name: Isobutanol
Reportable Quantity (RQ): 5000 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 1212 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: ISOBUTANOL

IATA

UN number: 1212 Class: 3 Packing group: III
Proper shipping name: Isobutanol

15. REGULATORY INFORMATION**SARA 302 Components**

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

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
iso-Butanol	78-83-1	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
iso-Butanol	78-83-1	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
iso-Butanol	78-83-1	1993-04-24

California Prop. 65 Components

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

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

Eye Dam.	Serious eye damage
Flam. Liq.	Flammable liquids

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H318 Causes serious eye damage.
H335 May cause respiratory irritation.
H336 May cause drowsiness or dizziness.
Skin Irrit. Skin irritation
STOT SE Specific target organ toxicity - single exposure

HMIS Rating

Health hazard: 2
Chronic Health Hazard:
Flammability: 3
Physical Hazard 0

NFPA Rating

Health hazard: 2
Fire Hazard: 3
Reactivity Hazard: 0

Further information

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Preparation Information

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Product Safety – Americas Region
1-800-521-8956

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