• SAFETY DATA SHEET

Version 7.0
Revision Date 03/16/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isobutyl butyrate

Product Number : W218715
Brand : Aldrich
CAS-No. : 539-90-2

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 3

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Short-term (acute) aquatic hazard	:	Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word	:	Warning
Hazard statements	:	H226 Flammable liquid and vapour. H401 Toxic to aquatic life.
Precautionary statements	:	**Prevention:** P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P233 Keep container tightly closed. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof electrical/ ventilating/ lighting equipment. P242 Use non-sparking tools. P243 Take action to prevent static discharges. P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. **Response:** P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. 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.	:	539-90-2

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Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Isobutyl butyrate	539-90-2*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.
TSC- the actual concentration or concentration range 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. Remove contact lenses.
If swallowed	:	After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.
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	:	Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Vapours are heavier than air and may spread along floors.

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Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

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. 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: 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

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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	:	Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection	:	required when vapours/aerosols are generated.
Recommended Filter type:	:	Filter type ABEK

The entrepeneur 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	:	Nitrile rubber
Break through time	:	10 min
Glove thickness	:	0.4 mm
Protective index	:	Splash contact
Manufacturer	:	Camatril® (KCL 730 / Aldrich Z677442, Size M)
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

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		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	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point	:	No data available
Boiling point/boiling range	:	315 - 316 °F / 157 - 158 °C Method: lit.
Flash point	:	115 °F / 46 °C Method: closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapor pressure	:	No data available
Relative vapour density	:	4.98 (Air = 1.0)
Relative density	:	No data available

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Density	:	0.861 g/cm3 (77 °F / 25 °C) Method: lit.
Water solubility	:	No data available
Partition coefficient: n-octanol/water	:	log Pow: 2.68
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	No data available
Molecular weight	:	144.21 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapour/air-mixtures are explosive at intense warming.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	Violent reactions possible with: Strong oxidizing agents
Conditions to avoid	:	Heating.
Incompatible materials	:	Strong oxidizing agents
Hazardous decomposition products	:	In the event of fire: see section 5

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SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - > 5,000 mg/kg
LD50 Oral - Rabbit - 9,520 mg/kg
Inhalation: No data available
Dermal: No data available
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 24 h

Serious eye damage/eye irritation
Remarks: No data available

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
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: ET5020000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Isobutyl butyrate:

Toxicity to daphnia and other aquatic invertebrates	:	NOEC (Daphnia magna (Water flea)): 3.17 mg/l Exposure time: 48 h Test Type: static test Method: OECD Test Guideline 202 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: butyl butyrate EC50 (Daphnia magna (Water flea)): 8.86 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: butyl butyrate
Toxicity to algae/aquatic plants	:	NOEC (Raphidocelis subcapitata (freshwater green alga)): 17.1 mg/l Exposure time: 72 h Test Type: static test Method: OECD Test Guideline 201 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: butyl butyrate EC50 (Pseudokirchneriella subcapitata): 27.4 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: butyl butyrate

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Persistence and degradability

Components:

Isobutyl butyrate:

Biodegradability	:	aerobic Inoculum: activated sludge, non-adapted Concentration: 30 mg/l Result: Readily biodegradable. Biodegradation: 77 % Exposure time: 28 d Method: OECD Test Guideline 301F GLP: yes Remarks: (ECHA)

Bioaccumulative potential

Components:

Isobutyl butyrate:

Bioaccumulation	:	Remarks: No data available
Partition coefficient: n-octanol/water	:	log Pow: 2.68

Mobility in soil

Components:

Isobutyl butyrate:

Stability in soil	:	Remarks: No data available

Other adverse effects

Product:

Ozone-Depletion Potential	:	Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

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.

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SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 3272
Proper shipping name	:	Esters, n.o.s. (Isobutyl butyrate)
Class	:	3
Packing group	:	III
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	366
Packing instruction (passenger aircraft)	:	355

IMDG-Code

UN number	:	UN 3272
Proper shipping name	:	ESTERS, N.O.S. (Isobutyl butyrate)
Class	:	3
Packing group	:	III
Labels	:	3
EmS Code	:	F-E, S-D
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 3272
Proper shipping name	:	Esters, n.o.s.
Class	:	3
Packing group	:	III
Labels	:	Class 3 - Flammable liquids
ERG Code	:	127
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.

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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
SARA 313	:	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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

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.
This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

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:

US TSCA	:	All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

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

SECTION 16. OTHER INFORMATION

Relevant changes since previous version

8. Exposure controls/personal protection

Full text of other abbreviations

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 - 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

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