

SAFETY DATA SHEET

Version 6.11
Revision Date 12/18/2024
Print Date 12/19/2024

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 1-Butanol
Product Number : 281549
Brand : Sigma-Aldrich
Index-No. : 603-004-00-6
CAS-No. : 71-36-3

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

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)

Flammable liquids : Category 3

Acute toxicity (Oral) : Category 4
Skin irritation : Category 2
Serious eye damage : Category 1
Specific target organ toxicity - single exposure : Category 3 (Respiratory system, Central nervous system)

GHS label elements

Hazard pictograms :



Signal Word : Danger

Hazard Statements : H226 Flammable liquid and vapor.
H302 Harmful if swallowed.
H315 Causes skin irritation.
H318 Causes serious eye damage.
H335 May cause respiratory irritation.
H336 May cause drowsiness or dizziness.

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.
P261 Avoid breathing mist or vapors.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
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 cau-

tiously 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.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS-No.	Concentration (% w/w)
n-butanol	71-36-3	>= 90 - <= 100

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this material safety data sheet to the doctor in attendance.
If inhaled : After inhalation: fresh air. Call in physician.
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. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
Most important symp- : The most important known symptoms and effects are

toms and effects, both acute and delayed : 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. FIRE-FIGHTING 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 : Flash back possible over considerable distance.

Combustible.

Vapors are heavier than air and may spread along floors.

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 : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

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 : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapors, 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.
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. Chemisorb®). 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.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

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.

Further information on storage stability : Handle and store under inert gas.
hygroscopic

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
n-butanol	71-36-3	TWA	20 ppm	ACGIH
		C	50 ppm 150 mg/m ³	NIOSH REL
		TWA	100 ppm 300 mg/m ³	OSHA Z-1

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 A (acc. to DIN 3181) for vapours of organic compounds

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 : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.4 mm
Protective index : Full contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Material : Chloroprene
Break through time : 120 min
Glove thickness : 0.65 mm
Protective index : Splash contact
Manufacturer : KCL 720 Camapren®

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).
Tightly fitting safety goggles
- Skin and body protection : Flame retardant antistatic protective clothing.
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : liquid, clear
- Color : colorless
- Odor : ethanolic
- Odor Threshold : 0.004 ppm
- pH : 7 (68 °F / 20 °C)
Concentration: 70 g/l
- Melting point/ range : -130 °F / -90 °C
- Boiling point/boiling range : 241 - 244 °F / 116 - 118 °C
- Flash point : 95 °F / 35 °C
(1,013 hPa)
Method: ISO 2719, Pensky-Martens 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 / : 11.2 %(V)

Upper flammability limit	
Lower explosion limit / Lower flammability limit	: Lower explosion limit 1.4 %(V)
Vapor pressure	: < 10 hPa (68 °F / 20 °C)
Relative vapor density	: 2.56 (68 °F / 20 °C) (Air = 1.0)
Relative density	: No data available
Density	: 0.81 g/mL (77 °F / 25 °C)
Solubility(ies)	
Water solubility	: 66 g/l (68 °F / 20 °C) pH: 7 Method: OECD Test Guideline 105 GLP: yes
Partition coefficient: n- octanol/water	: log Pow: 1 (77 °F / 25 °C) pH: 7 Method: OECD Test Guideline 117 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: 649 °F / 343 °C
Decomposition tempera- ture	: No data available
Viscosity	
Viscosity, dynamic	: 2.95 mPa.s (68 °F / 20 °C)
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Surface tension	: 69.9 mN/m, 1 g/l, 68 °F / 20 °C, OECD Test Guideline 115, GLP: yes
Molecular weight	: 74.12 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapor/air-mixtures are explosive at intense warming.
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 oxidising agents chromium(VI) oxide Exothermic reaction with: Alkali metals Alkaline earth metals Aluminum strong reducing agents Acid chlorides
Conditions to avoid	: Exposure to moisture. Heating.
Incompatible materials	: No data available
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 790 mg/kg

Remarks: Liver:Fatty liver degeneration.

Kidney, Ureter, Bladder:Other changes.

Blood:Other changes.

(RTECS)

Inhalation: No data available

LD50 Dermal - Rabbit - male - 3,430 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 2 h

Remarks: (ECHA)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irreversible effects on the eye

(OECD Test Guideline 405)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: Chinese hamster lung cells

Metabolic activation: without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

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.

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.

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

May cause respiratory irritation. - Respiratory Tract, Skin, Eyes

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

May cause drowsiness or dizziness.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: EO1400000

Central nervous system depression, Gastrointestinal disturbance, drying, cracking of the skin, Skin irritation, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

n-butanol:

Toxicity to fish	: LC50 (Pimephales promelas (fathead minnow)): 1,376 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 1,328 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata (green algae)): 225 mg/l Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: EC50 (Daphnia magna (Water flea)): 18 mg/l End point: reproduction rate Exposure time: 21 d Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes
Toxicity to microorganisms	: EC50 (Pseudomonas putida): 4,390 mg/l Exposure time: 17 h Test Type: static test Method: DIN 38421 TEIL 8

Persistence and degradability

Components:

n-butanol:

Biodegradability : aerobic
Concentration: 3 mg/l
Result: Readily biodegradable.
Biodegradation: 92 %
Exposure time: 20 d
Remarks: (ECHA)

BOD/ThOD : 33 %
Remarks: (IUCLID)

Bioaccumulative potential

Components:

n-butanol:

Bioaccumulation : Species: Oncorhynchus mykiss (rainbow trout)
Bioconcentration factor (BCF): 0.38
Exposure time: 24 h
Concentration: 921 mg/l

Partition coefficient: n-octanol/water : log Pow: 1 (77 °F / 25 °C)
pH: 7
Method: OECD Test Guideline 117
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

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).

Components:

n-butanol:

Results of PBT and vPvB assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

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 1120
Proper shipping name : Butanols
Class : 3
Packing group : III
Labels : Class 3 - Flammable liquids
Packing instruction (cargo : 366
aircraft)
Packing instruction (pas- : 355
senger aircraft)

IMDG-Code

UN number : UN 1120
Proper shipping name : BUTANOLS

Class : 3
Packing group : III
Labels : 3
EmS Code : F-E, S-D
Marine pollutant : no

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

Not applicable for product as supplied.

National regulation

49 CFR Road

UN/ID/NA number : UN 1120
Proper shipping name : Butanols

Class : 3
Packing group : III
Labels : Class 3 - Flammable liquids
ERG Code : 129
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

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
n-butanol	71-36-3	5000	5000
n-butanol	71-36-3	100	100 (F003)

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
Chronic Health Hazard

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

n-butanol 71-36-3 >= 90 - <= 100 %

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).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

n-butanol 71-36-3 >= 90 - <= 100 %

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water 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

n-butanol 71-36-3

Pennsylvania Right To Know

n-butanol 71-36-3

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 ingredients 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

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL : USA. NIOSH Recommended Exposure Limits
OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA : 8-hour, time-weighted average
NIOSH REL / C : Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA : 8-hour time weighted average

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 Harmonized 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 - In-

ventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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 - Organization 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 additional terms and conditions of sale. Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Revision Date : 12/18/2024

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

US / EN