

SAFETY DATA SHEET

Version 6.5
Revision Date 03/02/2024
Print Date 05/12/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 3-Methyl-1-butanol

Product Number : 320021

Brand : SIGALD

Index-No. : 603-006-00-7

CAS-No. : 123-51-3

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

Flammable liquids (Category 3), H226

Acute toxicity, Inhalation (Category 4), H332

Skin irritation (Category 2), H315

SIGALD - 320021

Page 1 of 11

Serious eye damage (Category 1), H318

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

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 Statements

H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.

Precautionary Statements

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.
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

Repeated exposure may cause skin dryness or cracking.

May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Isoamyl alcohol
Isopentyl alcohol

Formula : C₅H₁₂O
Molecular weight : 88.15 g/mol
CAS-No. : 123-51-3
EC-No. : 204-633-5
Index-No. : 603-006-00-7

Component	Classification	Concentration
Isoamyl alcohol		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H332, H315, H318, H335	<= 100 %

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material 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. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

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.

5.3 Advice for firefighters

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

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 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.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Isoamyl alcohol	123-51-3	TWA	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	125 ppm	USA. ACGIH Threshold Limit Values (TLV)
		ST	125 ppm 450 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 360 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 360 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	100 ppm 360 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	125 ppm 450 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face 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 protection

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).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

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).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 Dermatril® L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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.

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------|---|
| a) Appearance | Form: liquid, clear
Color: colorless |
|---------------|---|

b) Odor	No data available
c) Odor Threshold	No data available
d) pH	5.6 at 25 g/l at 20 °C (68 °F)
e) Melting point/freezing point	Melting point/range: -117 °C (-179 °F)
f) Initial boiling point and boiling range	130 °C 266 °F
g) Flash point	43.5 °C (110.3 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 8 %(V) Lower explosion limit: 1.2 %(V)
k) Vapor pressure	ca.3 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	3.04 - (Air = 1.0)
m) Density	0.809 g/mL at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.35 at 23 °C (73 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected.
p) Autoignition temperature	335 °C (635 °F) at 1,013 - 1,017 hPa - DIN 51794
q) Decomposition temperature	No data available
r) Viscosity	5.32 mm ² /s at 20 °C (68 °F) - (ECHA)
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Relative vapor density	3.04 - (Air = 1.0)
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SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .
Stable under recommended storage conditions.

SIGALD - 320021

Page 7 of 11

Test for peroxide formation before distillation or evaporation. Test for peroxide formation or discard after 1 year.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

rubber

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Acute toxicity estimate Inhalation - 11.1 mg/l - vapor

(Expert judgment)

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

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation - 24 h

Remarks: (RTECS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes.

Remarks: (External MSDS)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

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 system

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

Repeated dose toxicity - Rat - male - inhalation (vapor) - 7 - 14 Weeks

Remarks: (in analogy to similar products)
(ECHA)

The value is given in analogy to the following substances: n-Amyl alcohol

RTECS: EL5425000

prolonged or repeated exposure can cause:, Nausea, Headache, Vomiting

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - Oncorhynchus mykiss (rainbow trout) - 700 mg/l - 96 h (OECD Test Guideline 203) Remarks: (IUCLID)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia - 260 mg/l - 48 h Remarks: (IUCLID)
Toxicity to bacteria	EC50 - Pseudomonas putida - 2,500 mg/l - 17 h Remarks: (IUCLID)

12.2 Persistence and degradability

No data available

Theoretical oxygen demand	2,740 mg/g Remarks: (Lit.)
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Ratio BOD/ThBOD	55 % Remarks: (Lit.)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

SIGALD - 320021

Page 9 of 11

12.5 Results of PBT and vPvB assessment

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

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

DOT (US)

UN number: 1105 Class: 3 Packing group: III

Proper shipping name: Pentanols

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 1105 Class: 3 Packing group: III EMS-

No: F-E, S-D

Proper shipping name: PENTANOLS

IATA

UN number: 1105 Class: 3 Packing group: III

Proper shipping name: Pentanols

SECTION 15: Regulatory information

SARA 302 Components

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

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

Isoamyl alcohol

CAS-No.
123-51-3Revision Date
2007-03-01**Pennsylvania Right To Know Components**

Isoamyl alcohol

CAS-No.
123-51-3Revision Date
2007-03-01

SECTION 16: Other information**Further information**

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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