ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

3-Methyl-1-butanol

Revision Date:2025-03-01 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name	: 3-Methyl-1-butanol
CBnumber	: CB8852971
CAS	: 123-51-3
EINECS Number	: 204-633-5
Synonyms	: Isoamyl alcohol,3-Methyl-1-butanol

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word Warning

Precautionary statements

P405 Store locked up.

P403+P235 Store in a well-ventilated place. Keep cool.

P370+P378 In case of fire: Use … for extinction.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H335 May cause respiratory irritation

H332 Harmful if inhaled

H319 Causes serious eye irritation

H315 Causes skin irritation

H226 Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-Methyl-1-butanol
Synonyms	: Isoamyl alcohol,3-Methyl-1-butanol
CAS	: 123-51-3
EC number	: 204-633-5
MF	: C5H12O
MW	: 88.15

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides

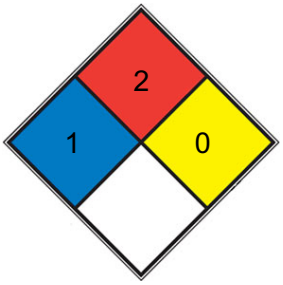
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704



■	HEALTH	1	Exposure would cause irritation with only minor residual injury (e.g. acetone, sodium bromate, potassium chloride)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. For personal protection see section 8.

Environmental precautions

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

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor 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.

Conditions for safe storage, including any incompatibilities

Store in cool place. 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.

Specific end use(s)

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

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SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

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) Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 30 min

Material tested:Dermatril? (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 EC 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.

Exposure limits

NIOSH REL: TWA 100 ppm (360 mg/m^3), IDLH 500 ppm; OSHA PEL: TWA 100 ppm; ACGIH TLV: TWA 100 ppm, STEL 125 ppm (adopted).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless liquid, clear
Odour	No data available
Odour Threshold	0.0017ppm
pH	5,6 at 25 g/l at 20 °C
Melting point/freezing point	-117 °C
Initial boiling point and boiling range	131 - 132 °C
Flash point	43 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 9 %(V) Lower explosion limit: 1,2 %(V)
Vapour pressure	3 hPa at 20 °C 23,6 hPa at 50 °C
Vapour density	3,04 - (Air = 1.0)
Relative density	0,809 g/mL at 20 °C
Water solubility	soluble
Partition coefficient: n-octanol/water	log Pow: 1,35 at 23 °C
Autoignition temperature	335 °C at 1.013 - 1.017 hPa
Decomposition temperature	No data available
Viscosity	5,32 mm2/s at 20 °C -
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	33.1 at 37 °C (Bylaite et al., 2004)

λmax	λ: 260 nm Amax: 0.06
	λ: 280 nm Amax: 0.06

Other safety information

Bulk density 808 kg/m3

Relative vapor density

3,04 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions. Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

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

Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

No data available

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

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.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory system

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

Additional Information

Repeated dose toxicity - Rat - male - inhalation (vapor) - 7 - 14 Weeks (in analogy to similar products) (ECHA)

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.

Toxicity

LD50 orally in rats: 7.07 ml/kg (Smyth)

SECTION 12: Ecological information

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)

Persistence and degradability

No data available

Theoretical oxygen demand

2.740 mg/g Remarks: (Lit.)

Ratio BOD/ThBOD 55 %

Remarks: (Lit.)

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Toxics Screening Level

The initial threshold screening level (ITSL) for isoamyl alcohol is 360 µg/m3 based on an 8 hr. averaging time.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Incompatibilities

Forms an explosive mixture with air. Contact with strong oxidizers and hydrogen trisulfide may cause fire and explosions. Incompatible with strong acids. Violent reaction with alkaline earth metals forming hydrogen, a flammable gas.

Waste Disposal

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. All federal, state, and local environmental regulations must be observed.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 1105 IMDG: 1105

UN proper shipping name

ADR/RID: PENTANOLS IMDG: PENTANOLS IATA: Pentanols

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

EC Inventory:Listed.

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

【1】CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

【2】ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

【3】ECHA - European Chemicals Agency, website: https://echa.europa.eu/

【4】eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

【6】Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

【7】HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

【8】IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

【9】IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

【10】Sigma-Aldrich, website: https://www.sigmaaldrich.com/