Chemical Safety Data Sheet MSDS / SDS

3-Methyl butynol

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name	: 3-Methyl butynol
CBnumber	: CB8852885
CAS	: 115-19-5
EINECS Number	: 204-070-5
Synonyms	: 2-methylbut-3-yn-2-ol,2-Methyl-3-butyn-2-ol

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 Danger

Precautionary statements

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

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

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

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

Continuerinsing.

Hazard statements

H225 Highly Flammable liquid and vapour

H302 Harmful if swallowed

H318 Causes serious eye damage

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-Methyl butynol
Synonyms	: 2-methylbut-3-yn-2-ol,2-Methyl-3-butyn-2-ol
CAS	: 115-19-5
EC number	: 204-070-5
MF	: C5H8O
MW	: 84.12

SECTION 4: First aid measures

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.

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

Carbon dioxide (CO2) Foam Dry powder

Unsuitable extinguishing media

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

Special hazards arising from the substance or mixture

Carbon oxides Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

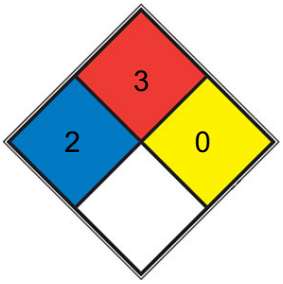
Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

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

NFPA 704



■	HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether, ammonium phosphate, iodine)
■	FIRE	3	Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, acetone)
■	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

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.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm Break through time: 480 min Material tested:Butoject? (KCL 898)

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 EN374 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: 0,4 mm Break through time: 30 min

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

Body Protection

Flame retardant antistatic protective clothing.

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 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless liquid
Odour	No data available
Odour Threshold	No data available
pH	7 (H_2O, 20℃)
Melting point/freezing point	Melting point/range: 2,6 °C - lit.
Initial boiling point and boiling range	104 °C - lit.
Flash point	20 °C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 16,6 %(V) Lower explosion limit: 1,8 %(V)
Vapour pressure	20 hPa at 20 °C
Vapour density	No data available
Relative density	0,868 g/mL at 25 °C - lit. No data available
Water solubility	completely miscible
Partition coefficient: n-octanol/water	log Pow: 0,32
Autoignition temperature	380 °C at 1.013,25 hPa
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 0,003 Pas at 20 °C
Explosive properties	Not explosive
Oxidizing properties	No data available

Other safety information

Surface tension 23,8 mN/m at 20 °C

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

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

Possibility of hazardous reactions

Risk of explosion with:

Copper alloys Copper

Risk of ignition or formation of inflammable gases or vapours with: Oxidizing agents

Exothermic reaction with:

acids

Conditions to avoid

Warming.

Incompatible materials

Copper, Copper alloys

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1.400 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 21,3 mg/l (OECD Test Guideline 403)

LD0 Dermal - Rabbit - male - 172 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 20 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: irritating - 8 d

Respiratory or skin sensitization

in vivo assay - Guinea pig

Result: Does not cause skin sensitization.

Germ cell mutagenicity

No data available Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471

Result: negative

Test Type: In vivo micronucleus test Species: Mouse

Application Route: Intraperitoneal Method: Mutagenicity (micronucleus test)

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

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

Toxicity

LD50 orally in Rabbit: 1420 mg/kg LD50 dermal Rat > 2000 mg/kg

---

SECTION 12: Ecological information

Toxicity

Toxicity to fish

static test LC50 - Leuciscus idus (Golden orfe) - 3.400 mg/l - 96 h (DIN 38412)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - > 500 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.)

Toxicity to algae

static test EC50 - Desmodesmus subspicatus (green algae) - > 500 mg/l - 72 h

Toxicity to bacteria

Respiration inhibition EC50 - Sludge Treatment - > 1.000 mg/l - 30 min

(ISO 8192)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 0 % - Not readily biodegradable.

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 3-Methyl butynol is 6.5 µg/m3 with annual averaging time.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

UN number

ADR/RID: 1987 IMDG: 1987 IATA: 1987

UN proper shipping name

ADR/RID: ALCOHOLS, N.O.S. (2-Methyl-3-butyn-2-ol) IMDG: ALCOHOLS, N.O.S. (2-Methyl-3-butyn-2-ol)

IATA: Alcohols, n.o.s. (2-Methyl-3-butyn-2-ol)

14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

14.5 Environmental hazards

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

14.6 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

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

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

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

EC Inventory:Listed.

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

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

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

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/