

SAFETY DATA SHEET according
to GB/T 16483 and GB/T 17519Version 8.0
Revision Date 24.01.2022
Print Date 24.04.2023
Date of first issue 24.01.2022SDS No. Sigma-Aldrich - W364620
Product Number Sigma-Aldrich - W364620**3-Methyl-2-butenal****SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-Methyl-2-butenal

Product Number : W364620
Brand : Sigma-Aldrich
CAS-No. : 107-86-8**1.2 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich (Shanghai) Trading Co.Ltd.
509 Renqing Road
Zhangjiang High Tech East Park, Pudong
SHANGHAI
201201 SHANGHAI
CHINA西格玛奥德里奇（上海）贸易有限公司
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邮政编码：201201Merck KGaA
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Fax : +86 21 6141-5567**1.3 Emergency telephone**

Emergency Phone # : +86 532 83889090

1.4 Relevant identified uses of the substance or mixture and uses advised againstIdentified uses : For R&D use only. Not for pharmaceutical, household or other
uses.**SECTION 2: Hazards identification****Summary of emergency**

clear, liquid light yellow Flammable liquid and vapor., Harmful if swallowed., May be harmful in contact with skin., Causes severe skin burns and eye damage., May cause an allergic skin reaction., Toxic if inhaled., Harmful to aquatic life. First aiders need to protect themselves., Show this material safety data sheet to the doctor in attendance. After inhalation: fresh air. Immediately call in physician., If breathing stops: immediately apply artificial respiration, if necessary also oxygen. In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower., Call a physician immediately. After eye contact: rinse out with plenty of water., Immediately call in ophthalmologist., Remove contact lenses. After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation)., Call a physician immediately., Do not attempt to neutralise. 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.

2.1 GHS Classification

Flammable liquids (Category 3), H226
 Acute toxicity, Oral (Category 4), H302
 Acute toxicity, Inhalation (Category 3), H331
 Acute toxicity, Dermal (Category 5), H313
 Skin corrosion/irritation (Category 1B), H314
 Serious eye damage/eye irritation (Category 1), H318
 Skin sensitization (Category 1), H317
 Short-term (acute) aquatic hazard (Category 3), H402

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 statement(s)

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H313	May be harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H331	Toxic if inhaled.
H402	Harmful to aquatic life.

Precautionary statement(s)

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 dust/ fume/ gas/ mist/ vapors/ spray.
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.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.

P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
Response	
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331 P303 + P361 + P353	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
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.
P312	Call a POISON CENTER/ doctor if you feel unwell.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P362 + P364	Take off contaminated clothing and wash it 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.

2.3 Physical and chemical hazards

H226 Flammable liquid and vapor.

2.4 Health hazards

H302 Harmful if swallowed.
H331 Toxic if inhaled.
H313 May be harmful in contact with skin.
H314 Causes severe skin burns and eye damage.
H318 Causes serious eye damage.
H317 May cause an allergic skin reaction.

2.5 Environmental hazards

H402 Harmful to aquatic life.

2.6 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Synonyms : 3,3-Dimethylacrylaldehyde
3,3-Dimethylacrolein
3-Methylcrotonaldehyde
Prenal

Formula : C₅H₈O
Molecular weight : 84.12 g/mol
CAS-No. : 107-86-8

Hazardous ingredients

Component	Classification	Concentration
3-Methyl-2-butenal	Flammable liquids Category 3; Acute toxicity Category 4; Acute toxicity Category 3; Acute toxicity Category 5; Skin corrosion/irritation Category 1B; Serious eye damage/eye irritation Category 1; Skin sensitization Category 1; Short-term (acute) aquatic hazard Category 3; H226, H302, H331, H313, H314, H318, H317, H402	<= 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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) 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.

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 carefully with liquid-absorbent material (e.g.

Chemizorb®). 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. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature

2 - 8 °C

Storage class

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

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

required

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.

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: clear, liquid
Color: light yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting | Melting point/range: -20 °C - (ECHA) |

	point/freezing point	
f)	Initial boiling point and boiling range	133 - 135 °C at 1,013 hPa
g)	Flash point	33 °C - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	9 hPa at 20 °C
l)	Vapor density	No data available
m)	Density	0.878 g/cm ³ at 20 °C
	Relative density	No data available
n)	Water solubility	110 g/l at 20 °C
o)	Partition coefficient: n-octanol/water	log Pow: 0.53 at 25 °C
p)	Autoignition temperature	145 °C at 1,013 hPa
q)	Decomposition temperature	No data available
r)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 1 mPa.s at 20 °C
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

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

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

Air
Heating.

10.4 Incompatible materials

Strong oxidizing agents, Strong bases

10.5 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 - male and female - 690 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 3.7 mg/l - vapor

(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - 3,400 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns. - 4 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes.

Remarks: (ECHA)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: May cause sensitization by skin contact.

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: in vivo assay

Species: Rat

Application Route: Oral

Method: OECD Test Guideline 486

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

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - NOAEL (No observed adverse effect level) - 77 mg/kg

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., 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 - Leuciscus idus (Golden orfe) - ca. 12.7 mg/l - 96 h (DIN 38412)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 13.5 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 22.4 mg/l - 92 h Remarks: (ECHA)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - > 1,000 mg/l - 30 min (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 80 - 90 % - Readily biodegradable. (ISO 14593)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

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

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

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14.1 UN number

ADR/RID: 2920

IMDG: 2920

IATA-DGR: 2920

14.2 UN proper shipping name

ADR/RID: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (3-Methyl-2-butenal)

IMDG: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (3-Methyl-2-butenal)

IATA-DGR: Corrosive liquid, flammable, n.o.s. (3-Methyl-2-butenal)

14.3 Transport hazard class(es)

ADR/RID: 8 (3)

IMDG: 8 (3)

IATA-DGR: 8 (3)

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

Strong oxidizing agents, Strong bases

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****National regulatory information****Other regulations**

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information**Full text of H-Statements referred to under sections 2 and 3.**

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H313	May be harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H402	Harmful to aquatic life.

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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

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