

SAFETY DATA SHEET

Version 6.1
Revision Date 05/07/2020
Print Date 05/28/2022

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

Product name : Methyl 2-oxobutanoate

Product Number : 713309
Brand : Aldrich
CAS-No. : 3952-66-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

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 number

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)**

Acute toxicity, Oral (Category 3), H301
Respiratory sensitisation (Category 1), H334
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

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)	
H301	Toxic if swallowed.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P304 + P341	IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/doctor.
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 - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	: C ₅ H ₈ O ₃
Molecular weight	: 116.12 g/mol
CAS-No.	: 3952-66-7

Component	Classification	Concentration
3-Methyl-2-oxo-butanoic acid		
	Acute Tox. 3; Resp. Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H301, H334, H402, H412	<= 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

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Combustible.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

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

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses 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.

Body Protection

Complete suit protecting against chemicals, 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 particle respirator type N99 (US) or type P2 (EN 143) 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.
Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Colour: light green, light yellow
b) Odour	characteristic
c) Odour Threshold	No data available
d) pH	2.7 at 100 g/l
e) Melting point/freezing point	-47 °C (-53 °F)
f) Initial boiling point and boiling range	154 °C 309 °F at 997 hPa - Tested according to Directive 92/69/EEC.
g) Flash point	50 °C (122 °F) - Tested according to Directive 92/69/EEC.
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	7.05 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapour density	No data available
m) Relative density	1.07 g/cm ³ at 20 °C (68 °F) - Tested according to Directive 92/69/EEC.
n) Water solubility	273 g/l at 20 °C (68 °F) - Tested according to Directive 92/69/EEC.
o) Partition coefficient: n-octanol/water	log Pow: 0.748 -
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

Surface tension	72 mN/m
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SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available

LD50 Dermal - Rat - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

- Mouse

Skin sensitisation

(OECD Test Guideline 406)

Germ cell mutagenicity

negative

Carcinogenicity

IARC: No component 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 component 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

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

Additional Information

Repeated dose toxicity - Rat - Gavage - No observed adverse effect level - 150 mg/kg

Subacute toxicity

RTECS: Not available

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

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SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish LC50 - Carassius auratus (goldfish) - 88 mg/l - 96 h
(Tested according to Directive 92/69/EEC.)

Toxicity to daphnia - Daphnia (water flea) - 15 mg/l - 48 h
and other aquatic
invertebrates

Toxicity to algae EC50 - SELENASTRUM - 44 mg/l

12.2 Persistence and degradability

Biodegradability

Remarks: Readily biodegradable, according to appropriate OECD test.

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life with long lasting 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. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquids, n.o.s. (3-Methyl-2-oxo-butanoic acid)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1993 Class: 3 Packing group: III EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (3-Methyl-2-oxo-butanoic acid)

IATA

UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquid, n.o.s. (3-Methyl-2-oxo-butanoic acid)

SECTION 15: Regulatory information

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

3-Methyl-2-oxo-butanoic acid	CAS-No. 3952-66-7	Revision Date
3-Methyl-2-oxo-butanoic acid	CAS-No. 3952-66-7	Revision Date

New Jersey Right To Know Components

3-Methyl-2-oxo-butanoic acid

CAS-No.
3952-66-7

Revision Date

SECTION 16: Other information

Further information

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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 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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