

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01
Supersedes Version 6.00***

Revision Date 07-Dec-2020
Issuing date 07-Dec-2020

SECTION 1: Identification

1.1. Product identifier

Identification of the
substance/preparation

3-Methylbutyric acid

CAS-No 503-74-2

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

Use of the Substance /
Preparation Intermediate
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Supplier **OQ Chemicals Corporation**
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA
Phone +1 346 378 7300

Product Information Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number NCEC +1 202 464 2554
available 24/7

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Skin corrosion/irritation Category 1B, H314
Serious eye damage/eye irritation Category 1, H318
Flammable liquid Category 4, H227
Environmental hazard Aquatic Acute 3; H402

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision

6.01

OSHA Specified Hazards Not applicable.

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

Hazard symbol(s)



Signal word

Danger

Hazard statements

H227: Combustible liquid
H314: Causes severe skin burns and eye damage.
H402: Harmful to aquatic life

Precautionary statements

Prevention

P210: Keep away from flames and hot surfaces. - No smoking.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P260: Do not breathe gas/mist/vapours.
P264: Wash hands thoroughly after handling.
P273: Avoid release to the environment.

Response

P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P363: Wash contaminated clothing before reuse.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310: Immediately call a POISON CENTER/doctor.***

Storage

P403 + P235: Store in a well ventilated place. Keep cool.
P405: Store locked up.

Disposal

P501: Dispose of contents/container in accordance with local regulation.

2.3. Other hazards

Vapour/air-mixtures are explosive at intense warming

SECTION 3: Composition / information on ingredients

Emergency telephone number
2 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

3.1. Substances

Component	CAS-No	Concentration (%)
Isovaleric acid	503-74-2	> 99,0

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Immediate medical attention is required.

Ingestion

Call a physician immediately. Do not induce vomiting without medical advice.

4.2. Most important symptoms and effects, both acute and delayed

Main symptoms

cough, dizziness, nausea, shortness of breath, unconsciousness, gastrointestinal discomfort.

Special hazard

Lung irritation, Lung oedema, Dermatitis.

4.3. Indication of any immediate medical attention and special treatment needed

General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. If ingested, flush stomach and compensate acidosis. In case of lung irritation, first treatment with cortisone spray.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

foam, dry chemical, carbon dioxide (CO₂), water spray

Unsuitable Extinguishing Media

Emergency telephone number
3 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision

6.01

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO₂)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapours are heavier than air and may spread along floors

Vapour/air-mixtures are explosive at intense warming

5.3. Advice for firefighters

Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting

Cool containers / tanks with water spray. Water run-off and vapor cloud may be corrosive. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.

For emergency responders: Personal protection see section 8.

6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant).

6.3. Methods and material for containment and cleaning up

Methods for containment

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

bases
amines
oxidizing agents

7.2. Conditions for safe storage, including any incompatibilities

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapour/air-mixtures are explosive at intense warming.

Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Keep at temperatures between 0 and 38 °C (32 and 100 °F).

Suitable material

stainless steel, aluminium

Unsuitable material

nickel, copper

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.

8.2. Exposure controls

Appropriate Engineering controls

Emergency telephone number
5 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Individual protection measures, such as personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	nitrile rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,55 mm
Break through time	> 480 min

Suitable material	polyvinylchloride
Evaluation	Information derived from practical experience
Glove thickness	approx 0,8 mm

Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (vapor or mist). Equipment should conform to NIOSH.***

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance liquid

Emergency telephone number
6 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision

6.01

Colour colourless
Odour unpleasant
Odour threshold 0,02 mg/m³
pH 3,1 (1 % in water @ 25 °C (77 °F)) DIN 19268***
Melting point/range - 23,8 °F (- 31 °C) (Pour point)
Method DIN ISO 3016***
Boiling point/range 353,3 °F (178,5 °C) @ 1 atm (101,3 kPa)
Method OECD 103***
Flash point 176 °F (80 °C) @ 1 atm (101,3 kPa)***
Method EN 22719
Evaporation rate No data available
Flammability (solid, gas) Does not apply, the substance is a liquid
Lower explosion limit 1,4 Vol %
Upper explosion limit 7,3 Vol %

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
1	0,1	0,001	20	68	DIN EN 13016-2***
6,6	0,66	0,007	50	122	DIN EN 13016-2***

Vapour density 3,5 (Air = 1) @ 20 °C (68 °F)

Relative density

Values	@ °C	@ °F	Method
0,9258	20	68	DIN 51757

Solubility 48 g/l @ 68 °F (20 °C), in water, OECD 105***

log Pow 1,7 @ 25 °C (77 °F) OECD 117***

Autoignition temperature 788 °F (420 °C) @ 988 hPa***

Method DIN 51794

Decomposition temperature No data available

Viscosity 2,437 mPa*s @ 68 °F (20 °C)

Method DIN 51562, dynamic

9.2. Other information

Molecular weight 102,13

Molecular formula C₅ H₁₀ O₂

log Koc 0,6045 calculated***

Dissociation constant pKa 4,7 @ 20 °C (68 °F), OECD 112***

Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

Refractive Index 1,403 @ 68 °F (20 °C)

Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

Surface tension 63,3 mN/m (1 g/l @ 20°C (68°F)), OECD 115***

SECTION 10: Stability and Reactivity

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerisation does not occur.

10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

10.5. Incompatible materials

bases, amines, oxidizing agents.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Eye contact, Skin contact, Inhalation, Ingestion

Isovaleric acid, CAS: 503-74-2

Main symptoms

cough, dizziness, nausea, shortness of breath, unconsciousness, gastrointestinal discomfort.

Target Organ Systemic Toxicant - Single exposure

Based on available data, the classification criteria are not met for:

STOT SE

Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:

STOT RE

Acute toxicity				
Isovaleric acid (503-74-2)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	~ 2500 mg/kg	rat male female	OECD 401
Dermal	LD50	> 2000 mg/kg	rabbit male female	OECD 402
Inhalative	LC0	2060 mg/m ³ (7 h)	rat	OECD 403

Isovaleric acid, CAS: 503-74-2

Emergency telephone number
8 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision

6.01

Assessment

Based on available data, the classification criteria are not met for:

Acute oral toxicity

Acute dermal toxicity

Acute inhalation toxicity

Irritation and corrosion

Isovaleric acid (503-74-2)

Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	1h
Respiratory tract***	rat***	slight irritation***	OECD 403***	7h***

Isovaleric acid, CAS: 503-74-2

Assessment

The available data lead to the classification given in section 2

Sensitization

Isovaleric acid (503-74-2)

Target Organ Effects	Species	Evaluation	Method	
Skin	Human experience	not sensitizing	OECD 406	1 %, in Petrolatum

Isovaleric acid, CAS: 503-74-2

Assessment

Based on available data, the classification criteria are not met for:

Skin sensitization

For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity

Isovaleric acid (503-74-2)

Type	Dose	Species	Method	
Subchronic toxicity	NOAEL: 4100 mg/kg/d (90d)	rat, male		Oral read across
Subchronic toxicity	NOAEL: 1068 mg/kg/d (90d)	rat, male	OECD 408	Oral read across
Subchronic toxicity	NOAEL: 1431 mg/kg/d (90d)	rat, female	OECD 408	Oral read across

Isovaleric acid, CAS: 503-74-2

Assessment

Based on available data, the classification criteria are not met for:

STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity

Isovaleric acid (503-74-2)

Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	read across
Mutagenicity		mouse	negative	OECD 474	read across

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

Developmental Toxicity	NOAEL 600 mg/kg/d	rat		OECD 414, Oral	Maternal toxicity, Developmental toxicity, Teratogenicity
Mutagenicity***		V79 cells, Chinese hamster***	negative***	OECD 476 (Mammalian Gene Mutation)***	read across***

Isovaleric acid, CAS: 503-74-2

CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

Evaluation

In vitro tests did not show mutagenic effects
Did not show reprotoxic effects in animal experiments

Isovaleric acid, CAS: 503-74-2

Aspiration toxicity

Due to the viscosity, this product does not present an aspiration hazard

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:
<http://echa.europa.eu/information-on-chemicals/registered-substances>.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Isovaleric acid (503-74-2)			
Species	Exposure time	Dose	Method
Pimephales promelas (fathead minnow)	96h	LC50: 77 mg/l	OECD 203 read across
Daphnia magna (Water flea)	48h	EC50: 51,25 mg/l	DIN 38412, part 11 read across
Pseudokirchneriella subcapitata	72h	EC50: 29,3 mg/l (Growth rate)***	OECD 201 read across
Tetrahymena pyriformis	40 h	IC50: 224 mg/l (Growth inhibition)	

Long term toxicity				
Isovaleric acid (503-74-2)				
Type	Species	Dose	Method	
Aquatic toxicity***	Pseudokirchneriella subcapitata***	NOEC: 12,6 mg/l (3d) Growth rate***	OECD 201 read across***	

12.2. Persistence and degradability

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

Isovaleric acid, CAS: 503-74-2

Biodegradation

58 - 66 % (8 d), activated sludge, aerobic, non-adapted, OECD 301 C.

Abiotic Degradation		
Isovaleric acid (503-74-2)		
Type	Result	Method
Hydrolysis***	not expected***	
Photolysis***	Half-life (DT50): 31,287 h***	calculated SRC AOP v1.92***

12.3. Bioaccumulative potential

Isovaleric acid (503-74-2)		
Type	Result	Method
log Pow	1,7 @ 25 °C (77 °F)***	measured, OECD 117
BCF	3,162 l/kg***	calculated

12.4. Mobility in soil

Isovaleric acid (503-74-2)		
Type	Result	Method
Surface tension	63,3 mN/m (1 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption***	Koc: 4,022***	calculated SRC PCKOCWIN v2.00***
Distribution to environmental compartments***	Air: 5,27% Soil: 57,1% Water: 37,6% Sediment: 0,0708%***	Calculation according Mackay, Level III***

12.5. Results of PBT and vPvB assessment

Isovaleric acid, CAS: 503-74-2

PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

12.6. Other adverse effects

Isovaleric acid, CAS: 503-74-2

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information

Emergency telephone number
11 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

SECTION 14: Transport information

D.O.T. (49CFR)

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (3-Methylbutyric acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user Emergency Response Guide	153

ICAO-TI / IATA-DGR

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (3-Methylbutyric acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (3-Methylbutyric acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user EmS	F-A, S-B

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

14.7. Transport in bulk according to Annex II not applicable
of MARPOL and the IBC Code

SECTION 15: Regulatory information

Federal and State Regulations

Components of the product are listed in the quoted regulations. For details please refer to the regulations directly. This list is not exhaustive, please check for other applicable regulations.

Federal Regulations

This product is listed on the TSCA inventory

State Regulations

Isovaleric acid, CAS: 503-74-2

MA RTK List
NJ RTK List
NY RTK List

International Inventories

Isovaleric acid, CAS: 503-74-2

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2079753 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-23545 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)
TCSI (TW)

SECTION 16: Other information

Revision Date 07-Dec-2020
Issuing date 07-Dec-2020

Hazard Rating Systems

NFPA (National Fire Protection Association)

Health Hazard	3
Fire Hazard	2
Reactivity	0

Emergency telephone number
13 / 14

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



3-Methylbutyric acid
10170

Version / Revision 6.01

HMS (Hazardous Material Information System)

Health Hazard	3
Flammability	2
Physical Hazard	0

Training advice

For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet

Information contained in this safety data sheet is based on OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet

Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the OQ homepage (www.chemicals.oq.com).

The use of a comma in section 3 and section 7 to 12 is the same as a period.

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

End of Safety Data Sheet