SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006 (REACh) Article 31, Annex II as amended

3-Methylbutyric acid
10170

Version / Revision	1	**Revision Date**	07-Nov-2023
Supersedes Version	-	**Issuing date**	07-Nov-2023

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

1.1. Product identifier

Identification of the substance/preparation **3-Methylbutyric acid**

CAS-No 503-74-2
EC No. 207-975-3
Registration number (REACh) 01-2119959864-19

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

Identified uses Transported isolated intermediate (1907/2006)
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking Identification
OQ Chemicals GmbH
Rheinpromenade 4A
D-40789 Monheim
Germany

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

1.4. Emergency telephone number

Emergency telephone number +44 (0) 1235 239 670 (UK)
available 24/7

National emergency telephone number
National Poisons Information Centre
+353 (0)1 809 2166
available to the public 8 am - 10 pm
+353 (0)1 809 2566
available 24/7 for medical professionals

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Skin corrosion/irritation Category 1B, H314
Serious eye damage/eye irritation Category 1, H318

Additional information
For full text of Hazard- and EU Hazard-statements see SECTION 16.

2.2. Label elements

Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).

Hazard pictograms

Signal word	**Danger**
Hazard statements	H314: Causes severe skin burns and eye damage.
Precautionary statements	P280: Wear protective gloves/protective clothing/eye protection/face protection. 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. 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.

2.3. Other hazards

Vapour/air-mixtures are explosive at intense warming

PBT and vPvB assessment	This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)
Endocrine disrupting assessments	The substance is not listed on the candidate list according to Art. 59(1), REACh. The substance was not assessed as having endocrine disrupting properties according to regulation 2017/2100/EU or 2018/605/EU.

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACh-No	1272/2008/EC	Concentration (%)
Isovaleric acid	503-74-2	01-2119959864-19	Skin Corr. 1B; H314 Eye Dam. 1; H318	> 99,0

For full text of Hazard- and EU Hazard-statements see SECTION 16.

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
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.

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.

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

Temperature class
T2

7.3. Specific end use(s)

Transported isolated intermediate (1907/2006)

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits European Union

No exposure limits established

Exposure limits Ireland

No exposure limits established.

DNEL & PNEC

This substance is registered as intermediate under strictly controlled conditions.

Isovaleric acid, CAS: 503-74-2
Workers
No data available

General population
No data available

Environment

PNEC aqua - freshwater	29,3 µg/l
PNEC aqua - marine water	2,93 µg/l
PNEC aqua - intermittent releases	0,293 mg/l
PNEC STP	22,4 mg/l
PNEC sediment - freshwater	117,3 mg/kg dw
PNEC sediment - marine water	11,7 mg/kg dw
PNEC Air	No hazard identified
PNEC soil	6,25 µg/kg dw
Secondary poisoning	No potential for bioaccumulation

8.2. Exposure controls

Special adaptations (REACh)

The substance has been registered as an transported isolated intermediate and must be handled throughout its life cycle under strictly controlled conditions in accordance with Article 18.4, REACH.

Appropriate Engineering controls
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.

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.
Equipment should conform to EN 166

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 A filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

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.

Additional advice
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 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	unpleasant
Odour threshold	0,02 mg/m³
Melting point/freezing point	- 31 °C (Pour point)
Method	DIN ISO 3016
Boiling point or initial boiling point and boiling range	178,5 °C @ 1013 hPa
Method	OECD 103
Flammability	Even if not classified as flammable, the product is capable of catching fire or being set on fire.
Lower explosion limit	1,4 Vol %
Upper explosion limit	7,3 Vol %
Flash point	80 °C @ 1013 hPa
Method	EN 22719
Autoignition temperature	420 °C @ 988 hPa
Method	DIN 51794
Decomposition temperature	No data available
pH	3,1 (1 % in water @ 25 °C (77 °F)) DIN 19268
Kinematic Viscosity	2,632 mm²/s @ 20 °C
Method	DIN 51562
Solubility	48 g/l @ 20 °C, in water, OECD 105
Partition coefficient n-octanol/water (log value)	1,7 @ 25 °C (77 °F) OECD 117

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

Density and/or relative density

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

Relative vapour density	3,5 (Air = 1) @ 20 °C (68 °F)
Particle characteristics	not applicable

9.2. Other information

Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
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
Refractive index	1,403 @ 20 °C
Surface tension	63,3 mN/m (1 g/l @ 20°C (68°F)), OECD 115
Evaporation rate	No data available

SECTION 10: Stability and Reactivity

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 hazard classes as defined in Regulation (EC) No 1272/2008

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

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/m³ (7 h)	rat	OECD 403

Isovaleric acid, CAS: 503-74-2
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
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
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
Aspiration toxicity
Due to the viscosity, this product does not present an aspiration hazard

11.2. Information on other hazards

Endocrine disrupting properties
The substance has not been identified as having endocrine disrupting properties in accordance with section 2.3.
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

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. Endocrine disrupting properties

The substance has not been identified as having endocrine disrupting properties in accordance with section 2.3.

12.7. Other adverse effects

Isovaleric acid, CAS: 503-74-2
No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information
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.
Hazardous waste according to European Waste Catalogue (EWC)

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

ADR/RID

14.1. UN number or ID 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	
ADR Tunnel restriction code	(E)
Classification Code	C3
Hazard Number	80

ADN ADN Container

14.1. UN number or ID 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	
Classification Code	C3
Hazard Number	80

ICAO-TI / IATA-DGR

14.1. UN number or ID 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 or ID 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
14.7. Maritime transport in bulk according to IMO instruments	not applicable

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI
not listed

DI 2012/18/EU (Seveso III)
Category not subject

VOC according to DI 2010/75/EU (Industry Emission Directive)

Component	Status
Isovaleric acid CAS: 503-74-2	regulated

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)

15.2. Chemical safety assessment

The Chemical Safety Report (CSR) is not required.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3
H314: Causes severe skin burns and eye damage.
H318: Causes serious eye damage.

Abbreviations
A table of terms and abbreviations can be found under the following link:
http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

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 Chemicals 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 Chemicals homepage (www.chemicals.oq.com).
The annex is not required because the substance is registered as an intermediate under REACh

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 Chemicals 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