

SAFETY DATA SHEET

according to REACH Regulation (EC) No. 1907/2006, as amended by UK REACH Regulations SI 2019/758



2-Methylbutyric acid 10070

Version / Revision 8.01
Supersedes Version 8.00***

Revision Date 25-Jan-2023
Issuing date 25-Jan-2023

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

1.1. Product identifier

Identification of the substance/preparation

2-Methylbutyric acid

CAS-No 116-53-0
EC No. 204-145-2

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

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)

Acute oral toxicity Category 4, H302
Acute dermal toxicity Category 4, H312
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

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Signal word

Danger

Hazard statements

H302: Harmful if swallowed.
H312: Harmful in contact with skin.
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	1272/2008/EC	Concentration (%)
2-Methylbutyric acid	116-53-0	Acute Tox. 4; H302 Acute Tox. 4; H312 Skin Corr. 1B; H314 Eye Dam. 1; H318 ATE = 1750 mg/kg (oral) ATE = 1367 mg/kg (dermal)	> 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.

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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.

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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.

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

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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 -18 and 38 °C (0 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 UK

No exposure limits established.

DNEL & PNEC

This substance is registered as intermediate under strictly controlled conditions.

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Workers

No data available

General population

No data available

Environment

No data available

8.2. Exposure controls

Special adaptations (REACH)

Not applicable.

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.

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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. Observe the exposure limits, clean exhaust air if needed. 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	No data available
Melting point/freezing point	- 90 °C @ 1013 hPa (Pour point)
Method	DIN ISO 3016

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Boiling point or initial boiling point and boiling range	177 °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	1,6 Vol %				
Upper explosion limit	7,3 Vol %				
Flash point	77 °C @ 1013 hPa				
Method	EN 22719				
Autoignition temperature	435 °C @ 1007 hPa				
Method	DIN 51794				
Decomposition temperature	No data available				
pH	3,1 (1 % in water @ 25 °C (77 °F)) DIN 19268				
Kinematic Viscosity	2,244 mm ² /s @ 20 °C				
Method	ASTM D445				
Solubility	45 g/l @ 20 °C, in water, OECD 105				
Partition coefficient n-octanol/water (log value)	1,8 @ 25 °C (77 °F) measured OECD 117				
Vapour pressure					
Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
1,68	0,168	0,002	20	68	DIN EN 13016-2
Density and/or relative density					
Values	@ °C	@ °F	Method		
0,9360	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
Dissociation constant	pKa 4,8 @ 20 °C (68 °F) OECD 112
Refractive index	1,405 @ 20 °C
Surface tension	64,2 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.

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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 Ingestion, Inhalation, Eye contact, Skin contact

Acute toxicity				
2-Methylbutyric acid (116-53-0)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	1750 mg/kg	rat, male/female	OECD 401
Dermal	LD50	2228 mg/kg	rabbit male	OECD 402
Dermal	LD50	1367 mg/kg	rabbit female	OECD 402
Inhalative	LC0	8375 mg/m ³ (6 h)	rat, male/female	OECD 403

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Assessment

The available data lead to the classification given in section 2

An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration

Irritation and corrosion				
2-Methylbutyric acid (116-53-0)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	3 min

2-Methylbutyric acid, CAS: 116-53-0

Assessment

The available data lead to the classification given in section 2

Available skin corrosion data suffice for classification of eye corrosion without further testing

For respiratory irritation, no data are available

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Assessment

Skin sensitization was not tested due to the corrosive properties of the substance

For respiratory sensitization, no data are available

2-Methylbutyric acid, CAS: 116-53-0

Assessment

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

STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity

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Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium Escherichia coli	negative	OECD 471 (Ames)	

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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

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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

no data available

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			
2-Methylbutyric acid (116-53-0)			
Species	Exposure time	Dose	Method
Danio rerio (Zebra fish)	96h	LC50: > 1000 mg/l	OECD 203
Bacteria / Sewage	24h	TTC: 1250 mg/l	ETAD Fermentation tube method
Daphnia magna (Water flea)	48h	LC50: 88,1 mg/l	OECD 202 read across
Pseudokirchneriella subcapitata	72h	EC50: 73,2 mg/l (Growth rate)	OECD 201 read across

Long term toxicity

2-Methylbutyric acid (116-53-0)			
Type	Species	Dose	Method
Aquatic toxicity	Pseudokirchneriella subcapitata	NOEC: 54,4 mg/l (3d) Growth inhibition	OECD 201 read across

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12.2. Persistence and degradability

2-Methylbutyric acid, CAS: 116-53-0

Biodegradation

67,9 % (10 d), Sewage, domestic, non-adapted, Readily biodegradable, OECD 301 D.

Abiotic Degradation		
2-Methylbutyric acid (116-53-0)		
Type	Result	Method
Hydrolysis	No data available	
Photolysis	No data available	

12.3. Bioaccumulative potential

2-Methylbutyric acid (116-53-0)		
Type	Result	Method
log Pow	1,8 @ 25 °C (77 °F)	measured, OECD 117
BCF	No data available	

12.4. Mobility in soil

2-Methylbutyric acid (116-53-0)		
Type	Result	Method
Surface tension	64,2 mN/m (1 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption	no data available	
Distribution to environmental compartments	no data available	

12.5. Results of PBT and vPvB assessment

2-Methylbutyric acid, CAS: 116-53-0

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

2-Methylbutyric acid, CAS: 116-53-0

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information

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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. (2-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 and Tanker

14.1. UN number or ID number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (2-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. (2-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
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14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (2-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

DI 1999/13/EC (VOC Guideline)

Component	Status
2-Methylbutyric acid CAS: 116-53-0	regulated

The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019 No. 758

Component	Status
2-Methylbutyric acid CAS: 116-53-0	The substance will not be pre-registered

For details and further information please refer to the original regulation.

International Inventories

2-Methylbutyric acid, CAS: 116-53-0

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2041452 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-23544 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)
TCSI (TW)

National regulatory information Great Britain

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Releases to air (Pollution Inventory Substances)

not subject

Releases to water (Pollution Inventory Substances)

not subject

Releases to sewer (Pollution Inventory Substances)

not subject

For details and further information please refer to the original regulation

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

H302: Harmful if swallowed.

H312: Harmful in contact with skin.

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 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 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

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