

Isobutyric acid

10290

Version / Revision3.01Revision Date12-Jan-2022Supersedes Version3.00***Issuing date12-Jan-2022

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

1.1. Product identifier

Identification of the substance/preparation

Isobutyric acid

CAS-No 79-31-2 **EC No.** 201-195-7

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

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

NCEC +1 202 464 2554

Local emergency telephone

number

+61 2 8014 4558 (Australia)

18000 74234 (Australia toll-free number)

+64 9 929 1483 (New Zealand)

0800 446 881 (New Zealand toll-free number)

+65 3158 1195 (Sri Lanka)

007 803 011 0293 (Indonesia toll-free number)

+60 3 6207 4347 (Malaysia)

001 800 120 666 751 (Thailand toll-free number)

+65 3158 1200 (Bangladesh) +63 2 8231 2149 (Philippines) +84 28 4458 2388 (Vietnam) +65 3165 2217 (Singapore)

available 24/7

SECTION 2: Hazards identification

Europe



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2.1. Classification of the substance or mixture

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

Flammable liquid Category 3, H226 Acute oral toxicity Category 4, H302 Acute dermal toxicity Category 3, H311 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

H226: Flammable liquid and vapour. **Hazard statements**

> H302: Harmful if swallowed. H311: Toxic in contact with skin.

H314: Causes severe skin burns and eye damage.

P280: Wear protective gloves/protective clothing/eye protection/face protection. **Precautionary statements**

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

Vapours may form explosive mixture with air

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic

(PBT), nor very persistent nor very bioaccumulating (vPvB)

USA



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2.1. Classification of the substance or mixture

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

Acute dermal toxicity Category 3, H311 Skin corrosion/irritation Category 1B, H314 Serious eye damage/eye irritation Category 1, H318 Flammable liquid Category 3, H226 Environmental hazard Aquatic Acute 3; H402

OSHA Specified Hazards No.

Not applicable.

2.2. Label elements

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

Hazard symbol(s)



Signal word

Danger

Hazard statements

H226: Flammable liquid and vapor. H311: Toxic in contact with skin.

H314: Causes severe skin burns and eye damage.

H402: Harmful to aquatic life

Precautionary statements

Prevention

P210: Keep away from heat, hot surfaces, sparks, open flames and other

ignition sources. No smoking. P233: Keep container tightly closed.

P240: Ground and bond container and receiving equipment.

P241: Use explosion-proof electrical/ ventilating/ lighting equipment.

P242: Use non-sparking tools.

P243: Take action to prevent static discharges.

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.

P302 + P352: IF ON SKIN: Wash with plenty of soap and water.

P361: Take off immediately all contaminated clothing and wash it before reuse. P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable

for breathing.

P310: Immediately call a POISON CENTER/doctor.

P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several



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minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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

Vapours may form explosive mixture with air

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACh-No	1272/2008/EC	Concentration (%)
Isobutyric acid	79-31-2	01-2119488973-18	Flam. Liq. 3; H226	> 99,5
-			Acute Tox. 4; H302	
			Acute Tox. 3; H311	
			Skin Corr. 1B; H314	
			Eye Dam. 1; H318	

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.

Eyes

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

Skin

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

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, abdominal pain, vomiting, shortness of breath, unconsciousness, discomfort.

Special hazard

Lung irritation, Lung oedema, Stomach perforation.

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.



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Treat symptomatically. If ingested, flush stomach and compensate acidosis.

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

Vapours may form explosive mixture with air

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).



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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 strong 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. Vapours may form explosive mixture with air.

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, Polyethylene

Unsuitable material

iron

Temperature class

T

7.3. Specific end use(s)

Intermediate under non-strictly controlled conditions Distribution of substance

SECTION 8: Exposure controls / personal protection

8.1. Control parameters



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Exposure limits European Union

No exposure limits established

Exposure limits Germany

No exposure limits established.

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

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.

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 butyl-rubber

Evaluation according to EN 374: level 6

Glove thickness approx 0,7 mm Break through time approx 480 min

Suitable material nitrile rubber

Evaluation according to EN 374: level 6

Glove thickness approx 0,55 mm Break through time > 480 min

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 (dust). Equipment should conform to NIOSH, EN or other applicable national standards.



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Environmental exposure controls

Use product only in closed system. 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.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

AppearanceliquidColourcolourlessOdourpungentOdour threshold8,1 ppm

pH 2,3 (50 % in water @ 25 °C (77 °F)) DIN 19268***

Melting point/range -64 °C (Freezing Point)***
Boiling point/range 156 °C @ 1013 hPa***

Flash point 56 - 62 °C Evaporation rate No data available

Flammability (solid, gas) Does not apply, the substance is a liquid

Lower explosion limit 1,6 Vol % **Upper explosion limit** 7,3 Vol %

Vapour pressure

Values [hPa] 2	Values [kPa] 0,2	Values [atm] 0,002	@ °C 20	@ °F 68	Method DIN EN
13	1.3	0.013	50	122	13016-2 DIN EN
13	1,3	0,013	50	122	13016-2

Vapour density 3,0 (Air = 1) @ 20 °C (68 °F)

Relative density

Values @ °C @ °F Method 0,948 20 68 DIN 51757 **Solubility** 618 g/l @ 20 °C, in water, OECD 105

log Pow 1,1 (measured), OECD 117 Autoignition temperature 455 °C @ 1018 hPa***

MethodDIN 51794Decomposition temperatureNo data availableViscosity1,32 mPa*s @ 20 °CMethodDIN 51562, dynamic

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

associated with oxidizing properties

Explosive propertiesDoes not apply, substance is not explosive. There are no chemical groups

associated with explosive properties

9.2. Other information

Molecular weight88,10Molecular formulaC4 H8 O2

log Koc 1,65 calculated***

Dissociation constant pKa 5 @ 21 °C (69,8 °F) OECD 112***

Refractive index 1,393 @ 20 °C

Surface tension 70,2 mN/m (1 g/l @ 20°C (68°F)), OECD 115



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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

Vapours may form explosive mixture with air.

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, strong 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 Inhalation, Eye contact, Skin contact, Ingestion

Acute toxicity				
Isobutyric acid (79-31-2)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	2230 mg/kg	rat, male/female	OECD 401
Dermal	LD50	474 mg/kg (24 h)	rabbit male***	OECD 402
Inhalative	LC0	9,59 mg/l (8 h)	rat, male/female	OECD 403

Isobutyric acid, CAS: 79-31-2

Assessment

The available data lead to the classification given in section 2

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

Acute oral toxicity

Acute inhalation toxicity

Irritation and corrosion				
Isobutyric acid (79-31-2	2)			
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	read across
Eyes	rabbit	corrosive		



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Isobutyric acid, CAS: 79-31-2

Assessment

The available data lead to the classification given in section 2 For respiratory irritation, no data are available

Isobutyric acid, CAS: 79-31-2

Assessment

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

Skin sensitization

For respiratory sensitization, no data are available

Isobutyric acid (79-31	 and prolonged toxicity -2) 	<i></i>		
Туре	Dose	Species	Method	
Subchronic toxicity	NOEL: 375 mg/kg/d (90d)***	rat, male/female	OECD 408 Oral	read across
Subchronic toxicity	NOAEC: 2500 ppm/ (14 weeks)***	d rat, male/female	OECD 413 Inhalation	read across

Isobutyric acid, CAS: 79-31-2

Assessment

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

STOT RE

	Carcinogenicity, Mutagenicity, Reproductive toxicity				
Isobutyric acid (79-31- Type		Species	Evaluation	Method	
Mutagenicity		CHO (Chinese Hamster Ovary) cells	negative	OECD 476 (Mammalian Gene Mutation)	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	
Mutagenicity		mouse	negative	OECD 474	read across in vivo
Reproductive toxicity	NOAEL: 2500 ppm***	rat		EPA OPPTS 870.3800 Inhalation***	read across
Developmental Toxicity	NOAEL 11,9 mg/l***	rat	Maternal toxicity Fetal toxicity Teratogenicity***	OECD 414, Inhalative	read across***
Developmental Toxicity	NOAEL 3 mg/l***	rabbit	Maternal toxicity	OECD 414, Inhalative	read across
Developmental Toxicity	NOAEL 11,9 mg/l***	rabbit	Teratogenicity Fetal toxicity, Embryotoxicity***	OECD 414, Inhalative	read across

Isobutyric acid, CAS: 79-31-2

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 mutagenic effects in animal experiments



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In the absence of specific alerts no cancer testing is required

Isobutyric acid, CAS: 79-31-2

Main symptoms

cough, abdominal pain, vomiting, shortness of breath, unconsciousness, 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

Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

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	Acute aquatic toxicity				
Isobutyric acid (79-31-2)	Isobutyric acid (79-31-2)				
Species	Exposure time	Dose	Method		
Daphnia magna (Water flea)	48h	EC50: 51,25 mg/l	DIN 38412, part 11		
Desmodesmus subspicatus	72h	EC50: 45,1 mg/l (Biomass)	DIN 38412, part 9		
Leuciscus idus (Golden orfe)	96h	LC50: 146,6 mg/l	DIN 38412, part 15		
Tetrahymena pyriformis	40 h	IC50: 190 mg/l (Growth inhibition)			

12.2. Persistence and degradability

Isobutyric acid, CAS: 79-31-2

Biodegradation

> 95 % (10 d), activated sludge, non-adapted, aerobic, OECD 302 B (Zahn-Wellens Test).

Abiotic Degradation			
Isobutyric acid (79-31-2)			
Туре	Result	Method	
Hydrolysis	not expected		
Photolysis	Half-life (DT50): 167 h***		

12.3. Bioaccumulative potential

Isobutyric acid (79-31-2)		
Type	Result	Method
log Pow	1,1 @ 25 °C (77 °F)***	measured, OECD 117
log BCF	0,5	calculated



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12.4. Mobility in soil

Isobutyric acid (79-31-2)		
Туре	Result	Method
Surface tension	70,2 mN/m (1 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption	log Koc: 1,65	calculated
Distribution to environmental	Air: 7,39 % Soil: 55 % Water: 37,5	calculated Fugacity Model Level III
compartments	% Sediment: 0,07 %	

12.5. Results of PBT and vPvB assessment

Isobutyric acid, CAS: 79-31-2
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

Isobutyric acid, CAS: 79-31-2

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

ICAO-TI / IATA-DGR

14.1. UN number 14.2. UN proper shipping nameUN 2529
Isobutyric acid

14.3. Transport hazard class(es)
Subsidiary Risk
8
14.4. Packing group
14.5. Environmental hazards

14.6. Special precautions for user no data available



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IMDG

UN 2529 **14.1. UN number** Isobutyric acid 14.2. UN proper shipping name

3 14.3. Transport hazard class(es) Subsidiary Risk 8 Ш 14.4. Packing group 14.5. Environmental hazards nο

14.6. Special precautions for user

F-E, S-C not applicable

14.7. Transport in bulk according to Annex

II of MARPOL and the IBC Code

ADR/RID

UN 2529 14.1. UN number 14.2. UN proper shipping name Isobutyric acid

14.3. Transport hazard class(es) 3 Subsidiary Risk 8 Ш 14.4. Packing group 14.5. Environmental hazards no

14.6. Special precautions for user

ADR Tunnel restriction code (D/E) Classification Code FC **Hazard Number** 38

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI

Isobutyric acid, CAS: 79-31-2

Classification Acute Tox. 4*; H312 Acute Tox. 4*; H302

GHS07 Exclamation mark **Hazard pictograms**

Warning Signal word **Hazard statements** H312, H302

DI 2012/18/EU (Seveso III)

Category Annex I, part 1:

P5a - c; depending on conditions

DI 1999/13/EC (VOC Guideline)

Component	Status
Isobutyric acid	regulated



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CAS: 79-31-2

International Inventories

Isobutyric acid, CAS: 79-31-2

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2011957 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-24875 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIOC (NZ)***
TCSI (TW)

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3

H226: Flammable liquid and vapour.

H302: Harmful if swallowed.

H311: Toxic 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).

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