SAFETY DATA SHEET

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

Isobutyric acid
10290

Version / Revision	6	**Revision Date**	27-Oct-2022
Supersedes Version	5.01***	**Issuing date**	27-Oct-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

Identified uses Intermediate under non-strictly controlled conditions
Distribution of substance
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)

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**

Hazard statements
H226: Flammable liquid and vapour.
H302: Harmful if swallowed.
H311: Toxic 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

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)

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 (%)
Isobutyric acid	79-31-2	Flam. Liq. 3; H226 Acute Tox. 4; H302 Acute Tox. 3; H311 Skin Corr. 1B; H314 Eye Dam. 1; H318 ATE = 474*** mg/kg (dermal)***	> 99,5

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, 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.

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).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Further info may be available in the appropriate Exposure scenarios in the annex to this SDS.

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
T1

7.3. Specific end use(s)

Intermediate under non-strictly controlled conditions
Distribution of substance
For specific end use information see the annex of this safety data sheet

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

Isobutyric acid, CAS: 79-31-2
Workers

DN(M)EL - long-term exposure - systemic effects - Inhalation	184 mg/m³
DN(M)EL - acute / short-term exposure - systemic effects - Inhalation	No hazard identified
DN(M)EL - long-term exposure - local effects - Inhalation	Hazard unknown (no further information necessary)
DN(M)EL - acute / short-term exposure - local effects - Inhalation	High hazard (no threshold derived)
DN(M)EL - long-term exposure - systemic effects - Dermal	3,75 mg/kg bw/day
DN(M)EL - acute / short-term exposure - systemic effects - Dermal	Hazard unknown (no further information necessary)
DN(M)EL - long-term exposure - local effects - Dermal	Hazard unknown (no further information necessary)
DN(M)EL - acute / short-term exposure - local effects - Dermal	High hazard (no threshold

DN(M)EL - local effects - eyes	derived) High hazard (no threshold derived)

General population

DN(M)EL - long-term exposure - systemic effects - Inhalation	92 mg/m³
DN(M)EL - acute / short-term exposure - systemic effects - Inhalation	No hazard identified
DN(M)EL - long-term exposure - local effects - Inhalation	Hazard unknown (no further information necessary)
DN(M)EL - acute / short-term exposure - local effects - Inhalation	High hazard (no threshold derived)
DN(M)EL - long-term exposure - systemic effects - Dermal	1,88 mg/kg bw/day
DN(M)EL - acute / short-term exposure - systemic effects - Dermal	Hazard unknown (no further information necessary)
DN(M)EL - long-term exposure - local effects - Dermal	Hazard unknown (no further information necessary)
DN(M)EL - acute / short-term exposure - local effects - Dermal	Hazard unknown (no further information necessary)
DN(M)EL - long-term exposure - systemic effects - Oral	1,88 mg/kg bw/day
DN(M)EL - acute / short-term exposure - systemic effects - Oral	No hazard identified
DN(M)EL - local effects - eyes	High hazard (no threshold derived)

Environment

PNEC aqua - freshwater	0,0451 mg/l
PNEC aqua - marine water	0,0045 mg/l
PNEC aqua - intermittent releases	0,451 mg/l
PNEC STP	19 mg/l
PNEC sediment - freshwater	0,364 mg/kg dw
PNEC sediment - marine water	0,0363 mg/kg dw
PNEC Air	No hazard identified
PNEC soil	0,0462 mg/kg dw
Secondary poisoning	No potential for bioaccumulation

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.

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	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 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
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.

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. For specific exposure controls see the annex to this safety data sheet.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	liquid***
Colour	colourless
Odour	pungent
Odour threshold	8,1 ppm
Melting point/freezing point	-64 °C (Freezing Point)
Method	DIN ISO 3016
Boiling point or initial boiling point and boiling range	156 °C @ 1013 hPa
Method	OECD 103
Flammability	Ignitable
Lower explosion limit	1,6 Vol %
Upper explosion limit	7,3 Vol %

Flash point	56 - 62 °C
Autoignition temperature	455 °C @ 1018 hPa
Method	DIN 51794
Decomposition temperature	No data available
pH	2,3 (50 % in water @ 25 °C (77 °F)) DIN 19268
Kinematic Viscosity	1,392 mm²/s @ 20 °C***
Method	DIN 51562***
Solubility	618 g/l @ 20 °C, in water, OECD 105
Partition coefficient n-octanol/water (log value)	1,1 (measured) OECD 117

Vapour pressure

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

Density and/or relative density

Values	@ °C	@ °F	Method
0,948	20	68	DIN 51757

Relative vapour density	3,0 (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	88,10
Molecular formula	C4 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
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

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

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)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	read across
Eyes	rabbit	corrosive		

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

Subacute, subchronic and prolonged toxicity				
Isobutyric acid (79-31-2)				
Type	Dose	Species	Method	
Subchronic toxicity	NOEL: 375 mg/kg/d (90d)	rat, male/female	OECD 408 Oral	read across
Subchronic toxicity	NOAEC: 2500 ppm/d (14 weeks)	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 (79-31-2)					
Type	Dose	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
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

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.
Isobutyric acid, CAS: 79-31-2
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			
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)		
Type	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

12.4. Mobility in soil

Isobutyric acid (79-31-2)		
Type	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 compartments	Air: 7,39 % Soil: 55 % Water: 37,5 % Sediment: 0,07 %	calculated Fugacity Model Level III

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. 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

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

ADR/RID

14.1. UN number or ID number	UN 2529
14.2. UN proper shipping name	Isobutyric acid
14.3. Transport hazard class(es)	3
Subsidiary Risk	8
14.4. Packing group	III
14.5. Environmental hazards	no
14.6. Special precautions for user	
ADR Tunnel restriction code	(D/E)
Classification Code	FC
Hazard Number	38

ADN ADN Container

14.1. UN number or ID number	UN 2529
14.2. UN proper shipping name	Isobutyric acid
14.3. Transport hazard class(es)	3
Subsidiary Risk	8
14.4. Packing group	III
14.5. Environmental hazards	no
14.6. Special precautions for user	

Classification Code	FC
Hazard Number	38

ICAO-TI / IATA-DGR

14.1. UN number or ID number	UN 2529
14.2. UN proper shipping name	Isobutyric acid
14.3. Transport hazard class(es)	3
Subsidiary Risk	8
14.4. Packing group	III
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number or ID number	UN 2529
14.2. UN proper shipping name	Isobutyric acid
14.3. Transport hazard class(es)	3
Subsidiary Risk	8
14.4. Packing group	III
14.5. Environmental hazards	no
14.6. Special precautions for user	
EmS	F-E, S-C
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

Isobutyric acid, CAS: 79-31-2

Classification	Acute Tox. 4*; H312 Acute Tox. 4*; H302
Hazard pictograms	GHS07 Exclamation mark
Signal word	Warning
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 CAS: 79-31-2	regulated

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

Component	Status

Isobutyric acid CAS: 79-31-2	The substance is/will be pre-registered

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

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)

National regulatory information Great Britain

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) has been generated. For Exposure Scenarios see the annex.

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 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

Annex to the extended Safety Data Sheet (eSDS)

General information

For specific information regarding the SPERC used please refer to the ESIG webpage
https://www.esig.org/reach-ges/environment/
Acute Health Hazard:
Local Human hazard:
Qualitative approach used to conclude safe use.

Other combinations of operational conditions may also be safe. Please contact OQ in case your local operational conditions differ from the ones described below and you are unsure if they are also safe

Operational conditions and risk management measures
Any measure to eliminate exposure should be considered
Containment of source except for short term exposure (e.g. taking sample)
Design closed system to allow for easy maintenance
If possible keep equipment under negative pressure
Control staff entry to work area
Ensure all equipment well maintained
Permit to work for maintenance work
Regular cleaning of equipment and work area
Supervision in place to check that the RMMs in place are being used correctly and OCs followed.
Training for staff on good practice
Procedures and training for emergency decontamination and disposal
Good standard of personal hygiene
Wear suitable eye protection, where direct contact (e.g. splashes) with substance is possible
Full skin coverage with appropriate light-weight barrier material
Substance/task appropriate gloves
Face-shield

Exposure scenario identification

1 Industrial use resulting in manufacture of another substance (use of intermediates)
2 Distribution of substance

Number of the ES 1

Short title of the exposure scenario
Industrial use resulting in manufacture of another substance (use of intermediates)

List of use descriptors

Sector of uses [SU]
SU3: Industrial uses: Uses of substances as such or in preparations at industrial sites
SU8: Manufacture of bulk, large scale chemicals (including petroleum products)
SU9: Manufacture of fine chemicals

Process categories [PROC]
PROC1: Use in closed process, no likelihood of exposure
PROC2: Use in closed, continuous process with occasional controlled exposure
PROC3: Use in closed batch process (synthesis or formulation)
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15: Use as laboratory reagent

Environmental release categories [ERC]
ERC6a: Industrial use resulting in manufacture of another substance (use of intermediates)

Product characteristics
Refer to attached safety data sheets

Processes and activities covered by the exposure scenario
Use as an intermediate (not related to Strictly Controlled Conditions). Includes incidental exposures during recycling/ recovery, material transfers, storage, sampling, associated laboratory activities, maintenance and loading (ncluding marine vessel/barge, road/rail car and bulk container).

Further explanations
Industrial use
Assumes use at not more than 20°C above ambient temperature (unless stated differently)

Contributing Scenarios

Number of the contributing scenario 1
Contributing exposure scenario controlling environmental exposure for ERC 6a

Further specification
SpERC ESVOC 6.1a.v1 release factors for (Sp)ERC were modified
assessment tool used: ECETOC TRA V2
Amounts used
Annual amount per site: 500 to
Daily amount per site: 1,6 to
Environment factors not influenced by risk management

River flow rate: 18000 m³/d
Technical conditions and measures at process level (source) to prevent release
Release fraction to air from process: 0.02 %
Release fraction to wastewater from process: 0.077 %
Release fraction to soil from process: 0.1%
Conditions and measures related to municipal sewage treatment plant
Size of municipal sewage system/ treatment plant (m³/d): 2000
The minimum grade of elimination in the sewage plant is (%): 87.35

Number of the contributing scenario **2**
Contributing exposure scenario controlling worker exposure for PROC 1

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid, vapour pressure < 0,5 kPa at STP
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 1 hand (240 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **3**
Contributing exposure scenario controlling worker exposure for PROC 2

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 2 hands (480 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **4**
Contributing exposure scenario controlling worker exposure for PROC 3

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 1 hand (240 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use

Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **5**
Contributing exposure scenario controlling worker exposure for
PROC 4

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 2 hands (480 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **6**
Contributing exposure scenario controlling worker exposure for
PROC 8a

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to 2 hands (960 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **7**
Contributing exposure scenario controlling worker exposure for
PROC 8b

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 2 hands (480 cm²)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **8**
Contributing exposure scenario controlling worker exposure for
PROC 9

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 2 hands (480 cm^2)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **9**
Contributing exposure scenario controlling worker exposure for PROC 15

Further specification
Assessment tool used: Ecetoc TRA V2 modified
Product characteristics
Liquid, vapour pressure < 0,5 kPa at STP
Covers percentage substance in the product up to 100 % (unless stated differently)
Frequency and duration of use
8 h (full shift)
Human factors not influenced by risk management
Area potentially exposed: corresponds to palm of 1 hand (240 cm^2)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Exposure estimation and reference to its source

Environment
PEC = predicted environmental concentration (local); RCR = risk characterisation ratio

Fresh Water (Pelagic)	PEC: 0.008 mg/l; RCR: 0.181
Fresh Water (Sediment)	PEC: 0.037 mg/kg dw; RCR: 0.989
Marine Water (Pelagic)	PEC: 0.001 mg/l; RCR: 0.181
Marine Water (Sediment)	PEC: 0.004 mg/kg dw; RCR: 0.989
Agricultural Soil	PEC: 0.002 mg/kg dw; RCR: 0.155
Sewage Treatment Plant (Effluent)	PEC: 0.081 mg/l; RCR: 0.004

Human exposure prediction (oral, dermal, inhalative)
Oral exposure is not expected to occur. EE(inhal): Estimated inhalative long-term exposure [mg/m^3]; EE(derm): Estimated dermal long-term exposure [mg/kg b.w./d]. The RMMs described above suffice to control risks for both local and systemic effects. Exposure estimates are given for either short-term or long-term exposure depending on which lead to more conservative risk characterisation ratios.

Proc 1	EE(inhal): 0.037 ; EE(derm): 0.069
Proc 2	EE(inhal): 3.671 ; EE(derm): 0.274
Proc 3	EE(inhal): 11.014 ; EE(derm): 0.069
Proc 4	EE(inhal): 18.356 ; EE(derm): 1.371
Proc 8a	EE(inhal): 36.713 ; EE(derm): 2.743
Proc 8b	EE(inhal): 18.356 ; EE(derm): 1.371
Proc 9	EE(inhal): 18.356 ; EE(derm): 1.371
Proc 15	EE(inhal): 18.356 ; EE(derm): 0.069

Risk characterisation
RCR(inhal): inhalative risk characterisation ratio; RCR(derm): dermal risk characterisation ratio; total RCR= RCR(inhal) +RCR(derm). Where required local and systemic effects were evaluated both for short-term and long-term exposure. The RCR's given correspond in each case to the most conservative calculated values.

Proc 1	RCR(inhal): 0.000 ; RCR(derm): 0.018
Proc 2	RCR(inhal): 0.020 ; RCR(derm): 0.073
Proc 3	RCR(inhal): 0.060 ; RCR(derm): 0.018
Proc 4	RCR(inhal): 0.100 ; RCR(derm): 0.366
Proc 8a	RCR(inhal): 0.200 ; RCR(derm): 0.731
Proc 8b	RCR(inhal): 0.100 ; RCR(derm): 0.366
Proc 9	RCR(inhal): 0.100 ; RCR(derm): 0.366
Proc 15	RCR(inhal): 0.100 ; RCR(derm): 0.018

Number of the ES 2

Short title of the exposure scenario
Distribution of substance

List of use descriptors

Sector of uses [SU]
SU3: Industrial uses: Uses of substances as such or in preparations at industrial sites
SU8: Manufacture of bulk, large scale chemicals (including petroleum products)
SU9: Manufacture of fine chemicals

Process categories [PROC]
PROC1: Use in closed process, no likelihood of exposure
PROC2: Use in closed, continuous process with occasional controlled exposure
PROC3: Use in closed batch process (synthesis or formulation)
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15: Use as laboratory reagent

Environmental release categories [ERC]
ERC1: Manufacture of substances

Product characteristics
Refer to attached safety data sheets

Further explanations
Industrial use
Human health hazard assessment:
see attached exposure scenario No: 1
Assumes use at not more than 20°C above ambient temperature (unless stated differently)

Contributing Scenarios

Number of the contributing scenario 1
Contributing exposure scenario controlling environmental exposure for ERC 1

Further specification
SpERC ESVOC 1.1b.v1 (ESVOC 3).
Amounts used
daily wide dispersive use: 0.666 to/d
Fraction of EU tonnage used in region: 1
Fraction of Regional tonnage used locally: 0.02
Amounts used (EU): 10000 to/a
Environment factors not influenced by risk management
River flow rate: 18000 m³/d Local freshwater dilution factor: 10 Local marine water dilution factor: 100
Technical conditions and measures at process level (source) to prevent release
Release fraction to air from process: 0.01 %
Release fraction to wastewater from process: 0.001 %
Release fraction to soil from process: 0%
Conditions and measures related to municipal sewage treatment plant
Size of municipal sewage system/ treatment plant (m³/d): 2000
The minimum grade of elimination in the sewage plant is (%): 87.35

Exposure estimation and reference to its source

Environment
PEC = predicted environmental concentration (local); RCR = risk characterisation ratio

Fresh Water (Pelagic)	PEC: 0.000 mg/l; RCR: 0.002
Fresh Water (Sediment)	PEC: 0.000 mg/kg dw; RCR: 0.009
Marine Water (Pelagic)	PEC: 0.000 mg/l; RCR: 0.002
Marine Water (Sediment)	PEC: 0.000 mg/kg dw; RCR: 0.09
Agricultural Soil	PEC: 0.000 mg/kg dw; RCR: 0.004
Sewage Treatment Plant (Effluent)	PEC: 0.00 mg/l; RCR: 0.000