SAFETY DATA SHEET

Isobutyric acid
10290

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
Registration number (REACH) 01-2119488973-18***

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

Identified uses
Intermediate under non-strictly controlled conditions

Uses advised against
None

1.3. Details of the supplier of the safety data sheet

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

Product Information
Product Stewardship
FAX: +49 (0)208 693 2053
email: psq@oxea-chemicals.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
SAFETY DATA SHEET

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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)

SECTION 3: Composition / information on ingredients

3.1. Substances

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>REACH-No</th>
<th>1272/2008/EC</th>
<th>Concentration (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isobutyric acid</td>
<td>79-31-2</td>
<td>01-2119488973-18** *</td>
<td>Flam. Liq. 3; H226 Acute Tox. 4; H302 Acute Tox. 3; H311 Skin Corr. 1B; H314 Eye Dam. 1; H318</td>
<td>&gt; 99,5</td>
</tr>
</tbody>
</table>

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**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Exposure limit</th>
<th>Hazard classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>DN(M)EL - long-term exposure - systemic effects - Inhalation</td>
<td>184 mg/m³</td>
<td>No hazard identified***</td>
</tr>
<tr>
<td>DN(M)EL - acute / short-term exposure - systemic effects - Inhalation</td>
<td></td>
<td>Hazard unknown (no further information necessary)***</td>
</tr>
<tr>
<td>DN(M)EL - long-term exposure - local effects - Inhalation</td>
<td></td>
<td>High hazard (no threshold derived)***</td>
</tr>
<tr>
<td>DN(M)EL - acute / short-term exposure - local effects - Inhalation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DN(M)EL - long-term exposure - systemic effects - Dermal</td>
<td>3,75 mg/kg bw/day</td>
<td>Hazard unknown (no further information available)***</td>
</tr>
<tr>
<td>DN(M)EL - acute / short-term exposure - systemic effects - Dermal</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---
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DN(M)EL - long-term exposure - local effects - Dermal
information necessary)***

DN(M)EL - acute / short-term exposure - local effects - Dermal
High hazard (no further information necessary)***

DN(M)EL - local effects - eyes
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

PNEC sediment - marine water
0,0363 mg/kg

PNEC Air
No hazard identified***

PNEC soil
0,0462 mg/kg

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
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**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.

<table>
<thead>
<tr>
<th>Suitable material</th>
<th>butyl-rubber</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaluation</td>
<td>according to EN 374: level 6</td>
</tr>
<tr>
<td>Glove thickness</td>
<td>approx 0.7 mm</td>
</tr>
<tr>
<td>Break through time</td>
<td>approx 480 min</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Suitable material</th>
<th>nitrile rubber</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaluation</td>
<td>according to EN 374: level 6</td>
</tr>
<tr>
<td>Glove thickness</td>
<td>approx 0.55 mm</td>
</tr>
<tr>
<td>Break through time</td>
<td>&gt; 480 min</td>
</tr>
</tbody>
</table>

**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**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>liquid</td>
</tr>
<tr>
<td>Colour</td>
<td>colourless</td>
</tr>
<tr>
<td>Odour</td>
<td>pungent</td>
</tr>
<tr>
<td>Odour threshold</td>
<td>8.1 ppm</td>
</tr>
<tr>
<td>pH</td>
<td>2.3 (50 % in water @ 25 °C (77 °F))</td>
</tr>
</tbody>
</table>
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Melting point/range  -64 °C (Pour point)
Boiling point/range  156 °C
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

<table>
<thead>
<tr>
<th>Values [hPa]</th>
<th>Values [kPa]</th>
<th>Values [atm]</th>
<th>@ °C</th>
<th>@ °F</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0,2</td>
<td>0,002</td>
<td>20</td>
<td>68</td>
</tr>
<tr>
<td>13</td>
<td>1,3</td>
<td>0,013</td>
<td>50</td>
<td>122</td>
</tr>
</tbody>
</table>

Method DIN EN 13016-2***

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

Relative density

<table>
<thead>
<tr>
<th>Values</th>
<th>@ °C</th>
<th>@ °F</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,948</td>
<td>20</td>
<td>68</td>
</tr>
</tbody>
</table>

Method DIN 51757

Solubility  618 g/l @ 20 °C, in water, OECD 105***

log Pow  1,1 (measured), OECD 117

Autoignition temperature  455 °C

Method DIN 51794

Decomposition temperature  No data available

Viscosity  1,32 mPa*s @ 20 °C

Method DIN 51562, dynamic

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

9.2. Other information

Molecular weight  88,10
Molecular formula  C4 H8 O2
Refractive index  1,393 @ 20 °C
Surface tension  70,2 mN/m (1 g/l @ 20°C (68°F)), OECD 115

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

<table>
<thead>
<tr>
<th>Isobutyric acid (79-31-2)</th>
<th>Routes of Exposure</th>
<th>Endpoint</th>
<th>Values</th>
<th>Species</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Oral</td>
<td>LD50</td>
<td>2230 mg/kg</td>
<td>rat, male/female</td>
<td>OECD 401</td>
</tr>
<tr>
<td></td>
<td>Dermal</td>
<td>LD50</td>
<td>474 mg/kg (24 h)</td>
<td>rabbit</td>
<td>OECD 402</td>
</tr>
<tr>
<td></td>
<td>Inhalative</td>
<td>LC0</td>
<td>9.59 mg/l (8 h)</td>
<td>rat, male/female</td>
<td>OECD 403</td>
</tr>
</tbody>
</table>

**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

<table>
<thead>
<tr>
<th>Isobutyric acid (79-31-2)</th>
<th>Target Organ Effects</th>
<th>Species</th>
<th>Result</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Skin</td>
<td>rabbit</td>
<td>corrosive</td>
<td>OECD 404</td>
</tr>
<tr>
<td></td>
<td>Eyes</td>
<td>rabbit</td>
<td>corrosive</td>
<td>read across</td>
</tr>
</tbody>
</table>

**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

<table>
<thead>
<tr>
<th>Isobutyric acid (79-31-2)</th>
<th>Type</th>
<th>Dose</th>
<th>Species</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Subchronic toxicity</td>
<td>NOAEL: 375 mg/kg</td>
<td>rat, male/female</td>
<td>OECD 408 Oral***</td>
</tr>
</tbody>
</table>

**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, 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)**

<table>
<thead>
<tr>
<th>Type</th>
<th>Dose</th>
<th>Species</th>
<th>Evaluation</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mutagenicity</td>
<td></td>
<td>CHO (Chinese Hamster Ovary) cells</td>
<td>negative</td>
<td>OECD 476 (Mammalian Gene Mutation)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Salmonella typhimurium</td>
<td>negative</td>
<td>OECD 471 (Ames)</td>
</tr>
<tr>
<td>Mutagenicity</td>
<td></td>
<td>mouse</td>
<td>negative</td>
<td>OECD 474</td>
</tr>
<tr>
<td>Reproductive toxicity</td>
<td></td>
<td>rat***</td>
<td></td>
<td>EPA OPPTS 870.3800</td>
</tr>
<tr>
<td>Developmental Toxicity</td>
<td></td>
<td>NOEC 11,9 mg/m³***</td>
<td>rat</td>
<td>OECD 414, Inhalative</td>
</tr>
<tr>
<td>Developmental Toxicity</td>
<td></td>
<td>NOEC 2,8 mg/m³***</td>
<td>rabbit</td>
<td>Maternal toxicity, OECD 414, Inhalative</td>
</tr>
<tr>
<td>Developmental Toxicity</td>
<td></td>
<td>NOEC 2,8 mg/m³***</td>
<td>rabbit</td>
<td>Fetal toxicity, OECD 414, Inhalative</td>
</tr>
<tr>
<td>Developmental Toxicity</td>
<td></td>
<td>NOEC 11,9 mg/m³***</td>
<td>rabbit</td>
<td>Teratogenicity, OECD 414, Inhalative</td>
</tr>
</tbody>
</table>

**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***

**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:
# SAFETY DATA SHEET

**Isobutyric acid**  
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---


## SECTION 12: Ecological information

### 12.1. Toxicity

**Acute aquatic toxicity**

<table>
<thead>
<tr>
<th>Isobytric acid (79-31-2)</th>
<th>Exposure time</th>
<th>Dose</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Daphnia magna</em> (Water flea)</td>
<td>48h</td>
<td>EC50: 51.25 mg/l</td>
<td>DIN 38412, part 11</td>
</tr>
<tr>
<td><em>Desmodesmus subspicatus</em></td>
<td>72h</td>
<td>EC50: 45.1 mg/l (Biomass)</td>
<td>DIN 38412, part 9</td>
</tr>
<tr>
<td><em>Leuciscus idus</em> (Golden orfe)</td>
<td>96h</td>
<td>LC50: 146.6 mg/l</td>
<td>DIN 38412, part 15</td>
</tr>
<tr>
<td><em>Tetrahymena pyriformis</em></td>
<td>40h</td>
<td>IC50: 190 mg/l (Growth inhibition)</td>
<td></td>
</tr>
</tbody>
</table>

### 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).

<table>
<thead>
<tr>
<th>Isobytric acid (79-31-2)</th>
<th>Type</th>
<th>Result</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Hydrolysis</em>**</td>
<td>not expected***</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Photolysis</em>**</td>
<td>No data available***</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 12.3. Bioaccumulative potential

<table>
<thead>
<tr>
<th>Isobytric acid (79-31-2)</th>
<th>Type</th>
<th>Result</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>log Pow***</td>
<td>1.1***</td>
<td>measured, OECD 117***</td>
<td></td>
</tr>
<tr>
<td>log BCF***</td>
<td>0.5***</td>
<td>calculated***</td>
<td></td>
</tr>
</tbody>
</table>

### 12.4. Mobility in soil

<table>
<thead>
<tr>
<th>Isobytric acid (79-31-2)</th>
<th>Type</th>
<th>Result</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension***</td>
<td>70.2 mN/m (1 g/l @ 20°C (68°F))***</td>
<td>OECD 115***</td>
<td></td>
</tr>
<tr>
<td>Adsorption/Desorption***</td>
<td>log Koc: 1.65***</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Distribution to environmental compartments***</td>
<td>Air: 7.39 % Soil: 55 % Water: 37.5 % Sediment: 0.07 %***</td>
<td></td>
<td></td>
</tr>
<tr>
<td>calculated Fugacity Model Level III***</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 12.5. Results of PBT and vPvB assessment

**Isobytric 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.

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 ***
14.2. UN proper shipping name *** Isobutyric acid
14.3. Transport hazard class(es) *** 3
   Subsidiary Risk *** 8
   *** III
14.4. Packing group ***
14.5. Environmental hazards ***
14.6. Special precautions for user
   ADR Tunnel restriction code (D/E)
   Classification Code FC
   Hazard Number 38

ADN

14.1. UN number ***
14.2. UN proper shipping name *** Isobutyric acid
14.3. Transport hazard class(es) *** 3
   Subsidiary Risk *** 8
   *** III
14.4. Packing group ***
14.5. Environmental hazards ***
14.6. Special precautions for user
   Classification Code FC
   Hazard Number 38
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Icao-Ti / Iata-Dgr

14.1. UN 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
*** 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. Transport in bulk according to Annex II of MARPOL and the IBC Code
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)

<table>
<thead>
<tr>
<th>Component</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isobutyric acid CAS: 79-31-2</td>
<td>regulated</td>
</tr>
</tbody>
</table>

International Inventories
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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:

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 Oxea 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
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information, other material safety data sheets or technical data sheets please consult the Oxea homepage (www.oxea-chemicals.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. Oxea 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
www.esig.org/en/regulatory-information/reach/ges-library

Acute Health Hazard:
Local Human hazard:
Qualitative approach used to conclude safe use.

Other combinations of operational conditions may also be safe. Please contact Oxea 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

<table>
<thead>
<tr>
<th>Number of the ES</th>
<th>Exposure scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Industrial use resulting in manufacture of another substance (use of intermediates)</td>
</tr>
<tr>
<td>2</td>
<td>Distribution of substance</td>
</tr>
</tbody>
</table>

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
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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 (including 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 (ESVOC 2) 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)
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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)
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<thead>
<tr>
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</tr>
</thead>
</table>

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.

<table>
<thead>
<tr>
<th>Number of the contributing scenario</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contributing exposure scenario controlling worker exposure for PROC 8a</td>
<td></td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Number of the contributing scenario</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contributing exposure scenario controlling worker exposure for PROC 8b</td>
<td></td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Number of the contributing scenario</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contributing exposure scenario controlling worker exposure for PROC 9</td>
<td></td>
</tr>
</tbody>
</table>

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.
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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 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.

Exposure estimation and reference to its source

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

<table>
<thead>
<tr>
<th>Environment</th>
<th>PEC</th>
<th>RCR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fresh Water (Pelagic)</td>
<td>0.008 mg/l; RCR: 0.181</td>
<td></td>
</tr>
<tr>
<td>Fresh Water (Sediment)</td>
<td>0.037 mg/kg dw; RCR: 0.989</td>
<td></td>
</tr>
<tr>
<td>Marine Water (Pelagic)</td>
<td>0.001 mg/l; RCR: 0.181</td>
<td></td>
</tr>
<tr>
<td>Marine Water (Sediment)</td>
<td>0.004 mg/kg dw; RCR: 0.989</td>
<td></td>
</tr>
<tr>
<td>Agricultural Soil</td>
<td>0.002 mg/kg dw; RCR: 0.155</td>
<td></td>
</tr>
<tr>
<td>Sewage Treatment Plant (Effluent)</td>
<td>0.081 mg/l; RCR: 0.004</td>
<td></td>
</tr>
</tbody>
</table>

Human exposure prediction (oral, dermal, inhalative)
Oral exposure is not expected to occur. EE(inhal): Estimated inhalative long-term exposure [mg/m³]; 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.

<table>
<thead>
<tr>
<th>Procedure</th>
<th>EE(inhal)</th>
<th>EE(derm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proc 1</td>
<td>0.037</td>
<td>0.069</td>
</tr>
<tr>
<td>Proc 2</td>
<td>3.671</td>
<td>0.274</td>
</tr>
<tr>
<td>Proc 3</td>
<td>11.014</td>
<td>0.069</td>
</tr>
<tr>
<td>Proc 4</td>
<td>18.356</td>
<td>1.371</td>
</tr>
<tr>
<td>Proc 8a</td>
<td>36.713</td>
<td>2.743</td>
</tr>
<tr>
<td>Proc 8b</td>
<td>18.356</td>
<td>1.371</td>
</tr>
<tr>
<td>Proc 9</td>
<td>18.356</td>
<td>1.371</td>
</tr>
<tr>
<td>Proc 15</td>
<td>18.356</td>
<td>0.069</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Procedure</th>
<th>RCR(inhal)</th>
<th>RCR(derm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proc 1</td>
<td>0.000</td>
<td>0.018</td>
</tr>
<tr>
<td>Proc 2</td>
<td>0.020</td>
<td>0.073</td>
</tr>
<tr>
<td>Proc 3</td>
<td>0.060</td>
<td>0.018</td>
</tr>
<tr>
<td>Proc 4</td>
<td>0.100</td>
<td>0.366</td>
</tr>
<tr>
<td>Proc 8a</td>
<td>0.200</td>
<td>0.731</td>
</tr>
<tr>
<td>Proc 8b</td>
<td>0.100</td>
<td>0.366</td>
</tr>
<tr>
<td>Proc 9</td>
<td>0.100</td>
<td>0.366</td>
</tr>
</tbody>
</table>
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Proc 15
RCR(inhal): 0.100 ; RCR(derm): 0.018

Number of the ES 2

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

<table>
<thead>
<tr>
<th>Environment</th>
<th>PEC (mg/l)</th>
<th>RCR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fresh Water (Pelagic)</td>
<td>0.000</td>
<td>0.002</td>
</tr>
<tr>
<td>Fresh Water (Sediment)</td>
<td>0.000</td>
<td>0.009</td>
</tr>
<tr>
<td>Marine Water (Pelagic)</td>
<td>0.000</td>
<td>0.002</td>
</tr>
<tr>
<td>Marine Water (Sediment)</td>
<td>0.000</td>
<td>0.09</td>
</tr>
<tr>
<td>Agricultural Soil</td>
<td>0.000</td>
<td>0.004</td>
</tr>
<tr>
<td>Sewage Treatment Plant (Effluent)</td>
<td>0.00</td>
<td>0.000</td>
</tr>
</tbody>
</table>