

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: **1HA9**  
Version: **GHS 3.0 en**  
Replaces version of: 2024-03-02  
Version: (GHS 2)

date of compilation: 2021-02-02  
Revision: 2024-04-08

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

### 1.1 Product identifier

Identification of the substance	<b>Isobutyric acid <math>\geq 99\%</math>, for synthesis</b>
Article number	1HA9
CAS number	79-31-2

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

Relevant identified uses:	Laboratory and analytical use Laboratory chemical
Uses advised against:	Do not use for squirting or spraying. Do not use for products which come into direct contact with the skin. Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0  
**Telefax:** +49 (0) 721 - 56 06 149  
**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification acc. to GHS

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: **1HA9**

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	3	Flam. Liq. 3	H226
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.1D	Acute toxicity (dermal)	3	Acute Tox. 3	H311
3.2	Skin corrosion/irritation	1B	Skin Corr. 1B	H314
3.3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

For full text of abbreviations: see SECTION 16

### The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis. The product is combustible and can be ignited by potential ignition sources.

## 2.2 Label elements

### Labelling

#### Signal word

**Danger**

#### Pictograms

GHS02, GHS05,  
GHS06



#### 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

##### Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
P260 Do not breathe dusts or mists  
P280 Wear protective gloves/protective clothing

##### Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of soap and water  
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

##### Precautionary statements - storage

P403+P235 Store in a well-ventilated place. Keep cool

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: 1HA9

### 2.3 Other hazards

#### Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

#### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Isobutyric acid
Molecular formula	$C_4H_8O_2$
Molar mass	88.11 g/mol
CAS No	79-31-2

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off immediately all contaminated clothing.

#### Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure.

#### Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

#### Following ingestion

Rinse mouth immediately and drink plenty of water. Rinse mouth with water (only if the person is conscious). Call a physician immediately. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

### 4.2 Most important symptoms and effects, both acute and delayed

Headache, Nausea, Vomiting, Corrosion, Risk of blindness, Gastric perforation, Risk of serious damage to eyes

### 4.3 Indication of any immediate medical attention and special treatment needed

none

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



**Isobutyric acid ≥99 %, for synthesis**

article number: **1HA9**

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours may form explosive mixtures with air.

#### Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures



#### For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

### 6.3 Methods and material for containment and cleaning up

#### Advice on how to contain a spill

Covering of drains.

#### Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: **1HA9**

### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation. Use extractor hood (laboratory). Handle and open container with care. Clear contaminated areas thoroughly.

#### Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

#### Advice on general occupational hygiene

Thorough skin-cleansing after handling the product. When using do not smoke.

### 7.2 Conditions for safe storage, including any incompatibilities

Store in a well-ventilated place. Keep container tightly closed.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

Store locked up. Ground/bond container and receiving equipment.

#### Ventilation requirements

Use local and general ventilation.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

#### Human health values

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: 1HA9

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	184 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	3.75 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

### Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0.045 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.004 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	19 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0.364 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.036 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.046 mg/kg	terrestrial organisms	soil	short-term (single instance)

## 8.2 Exposure controls

### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggle with side protection. Wear face protection.

#### Skin protection



#### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • type of material

Butyl caoutchouc (butyl rubber)

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid ≥99 %, for synthesis

article number: **1HA9**

- **material thickness**

≥0,5 mm

- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	disagreeable - stinging
Odour threshold	8.1 ppm
Melting point/freezing point	-64 °C (ECHA)
Boiling point or initial boiling point and boiling range	156 °C at 1,013 hPa (ECHA)
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	1.6 vol% (LEL) - 7.3 vol% (UEL)
Flash point	56 – 62 °C at 1,013 hPa (c.c.)
Auto-ignition temperature	455 °C at 1,018 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	2.3 (in aqueous solution: 500 g/l, 25 °C)
Kinematic viscosity	1.395 mm <sup>2</sup> /s at 20 °C
Dynamic viscosity	1.322 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	618 g/l at 20 °C (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	1.1 (pH value: 3, 25 °C) (ECHA)

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: **1HA9**

Vapour pressure	2 hPa at 20 °C
<u>Density and/or relative density</u>	
Density	0.948 g/cm <sup>3</sup> at 20 °C (ECHA)
Relative vapour density	Information on this property is not available.
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none
<b>9.2 Other information</b>	
Information with regard to physical hazard classes:	There is no additional information.
Other safety characteristics:	
Surface tension	70.2 mN/m (20 °C) (ECHA)

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

It's a reactive substance. Risk of ignition.

#### If heated

Risk of ignition. Vapours may form explosive mixtures with air.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** strong oxidiser, Amines, Nitriles, Strong alkali

### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

### 10.5 Incompatible materials

different metals, aluminium, zinc

#### Release of flammable materials with

Metals (due to the release of hydrogen in an acid/alkaline medium).

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.



# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid ≥99 %, for synthesis

article number: 1HA9

### SECTION 11: Toxicological information

#### 11.1 Information on toxicological effects

##### Classification acc. to GHS

##### Acute toxicity

Harmful if swallowed. Toxic in contact with skin.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	2,230 mg/kg	rat	OECD 401	ECHA
dermal	LD50	474 mg/kg	rabbit	OECD 402	

##### Skin corrosion/irritation

Causes severe skin burns and eye damage.

##### Serious eye damage/eye irritation

Causes serious eye damage.

##### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

##### Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

##### Carcinogenicity

Shall not be classified as carcinogenic.

##### Reproductive toxicity

Shall not be classified as a reproductive toxicant.

##### Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

##### Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

##### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

##### Symptoms related to the physical, chemical and toxicological characteristics

###### • If swallowed

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

###### • If in eyes

causes burns, Causes serious eye damage, risk of blindness

###### • If inhaled

nausea, headache

###### • If on skin

causes severe burns, causes poorly healing wounds

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: 1HA9

### • Other information

none

### 11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 12: Ecological information

### 12.1 Toxicity

Harmful to aquatic life.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	146.6 mg/l	fish	ECHA	96 h
EC50	51.25 mg/l	aquatic invertebrates	ECHA	48 h

### 12.2 Persistence and degradability

Theoretical Oxygen Demand: 1.816 mg/mg  
Theoretical Carbon Dioxide: 1.998 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1.1 (pH value: 3, 25 °C) (ECHA)
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### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### Sewage disposal-relevant information

Do not empty into drains.

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid ≥99 %, for synthesis

article number: **1HA9**

### Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### Relevant provisions relating to waste(Basel Convention)

#### Properties of waste which render it hazardous

**H3** Flammable liquids

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

## SECTION 14: Transport information

### 14.1 UN number

<b>UN RTDG</b>	UN 2529
IMDG-Code	UN 2529
ICAO-TI	UN 2529

### 14.2 UN proper shipping name

<b>UN RTDG</b>	ISOBUTYRIC ACID
IMDG-Code	ISOBUTYRIC ACID
ICAO-TI	Isobutyric acid

### 14.3 Transport hazard class(es)

<b>UN RTDG</b>	3 (8)
IMDG-Code	3 (8)
ICAO-TI	3 (8)

### 14.4 Packing group

<b>UN RTDG</b>	III
IMDG-Code	III
ICAO-TI	III

### 14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

### 14.6 Special precautions for user

There is no additional information.

### 14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

### 14.8 Information for each of the UN Model Regulations

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: 1HA9

### Transport information National regulations Additional information (UN RTDG)

UN number	2529
Class	3
Subsidiary risk(s)	8
Packing group	III
Danger label(s)	3+8
Special provisions (SP)	- UN RTDG
Excepted quantities (EQ)	E1 UN RTDG
Limited quantities (LQ)	5 L UN RTDG
Emergency Action Code	2W

### International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	ISOBUTYRIC ACID
Particulars in the shipper's declaration	UN2529, ISOBUTYRIC ACID, 3 (8), III, 56°C c.c.
Marine pollutant	-
Danger label(s)	3+8
Special provisions (SP)	-
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
EmS	F-E, S-C
Stowage category	A

### International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name	Isobutyric acid
Particulars in the shipper's declaration	UN2529, Isobutyric acid, 3 (8), III
Danger label(s)	3+8
Excepted quantities (EQ)	E1
Limited quantities (LQ)	1 L

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid ≥99 %, for synthesis

article number: 1HA9

### SECTION 15: Regulatory information

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

There is no additional information.

##### National regulations(Australia)

##### Australian Inventory of Chemical Substances(AICS)

Substance is listed.

##### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

##### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

##### Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

#### 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid ≥99 %, for synthesis

article number: 1HA9

### SECTION 16: Other information

#### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.2		Pictograms: change in the listing (table)	yes
2.2		Hazard statements: change in the listing (table)	yes
14.8	Particulars in the shipper's declaration: UN2529, ISOBUTYRIC ACID, 3 (8), III	Particulars in the shipper's declaration: UN2529, ISOBUTYRIC ACID, 3 (8), III, 56°C c.c.	yes

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UEL	Upper explosion limit (UEL)

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Isobutyric acid $\geq 99\%$ , for synthesis

article number: **1HA9**

Abbr.	Descriptions of used abbreviations
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

### Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
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.

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.