

Phenyl isothiocyanate PEPTIPURE® ≥99 %, for biochemistry

article number: **7296** Version: **3.0 en** Replaces version of: 2023-02-02 Version: (2) date of compilation: 2021-02-18 Revision: 2023-07-03

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

1.1 Product identifier

Identification of the substance	Phenyl isothiocyanate PEPTIPURE® ≥99 %, for biochemistry			
Article number	7296			
EC number	203-138-1			
CAS number 103-72-0				
Pelevant identified uses of the substance or mix	vture and uses advised against			

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

Relevant identified uses:	Isolated intermediate
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 in- to 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 **Website:** www.carlroth.de

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

e-mail (competent person):

sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

acc. to Regulation (EC) No. 1907/2006 (REACH)



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Classification acc. to GHS					
Section	ection Hazard class		Hazard class and category	Hazard statement	
3.10	O Acute toxicity (oral)		Acute Tox. 3	H301	
3.2	3.2 Skin corrosion/irritation		Skin Corr. 1B	H314	
3.4R	3.4R Respiratory sensitisation		Resp. Sens. 1B	H334	
3.4S Skin sensitisation		1B	Skin Sens. 1B	H317	
4.1A	4.1A Hazardous to the aquatic environment - acute hazard		Aquatic Acute 1	H400	
4.1C	4.1C Hazardous to the aquatic environment - chronic hazard		Aquatic Chronic 1	H410	

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. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling

Signal word Danger

Pictograms

GHS05, GHS06, GHS08, GHS09



H301	Toxic if swallowed
H314	Causes severe skin burns and eye damage
H317	May cause an allergic skin reaction
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
H410	Very toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P280 Wear protective gloves/eye protection

Precautionary statements - response

P302+P352	IF ON SKIN: Wash with plenty of water
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing

2.3 Other hazards

This material is combustible, but will not ignite readily.

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 (EDC) in a concentration of \geq 0,1%.

acc. to Regulation (EC) No. 1907/2006 (REACH)



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SECTION 3: Composition/information on ingredients

3.1	Substances			
	Name of substance	Phenyl isothiocyanate		
	Molecular formula	C ₇ H₅NS		
	Molar mass	135,2 ^g / _{mol}		
	CAS No	103-72-0		
	EC No	203-138-1		

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	87 ^{mg} / _{kg}	oral

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

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. In case of skin reactions, consult a physician.

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. 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

Corrosion, Breathing difficulties, Cough, Risk of blindness, Gastric perforation, Vomiting, Allergic reactions, Nausea

4.3 Indication of any immediate medical attention and special treatment needed

none

acc. to Regulation (EC) No. 1907/2006 (REACH)



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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulphur oxides (SOx), Hydrogen cyanide (HCN, prussic acid)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Do not allow firefighting water to enter drains or water courses. 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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Do not breathe vapour/spray.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

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.

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.

acc. to Regulation (EC) No. 1907/2006 (REACH)

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. 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.

Measures to protect the environment

Avoid release to the environment.

Advice on general occupational hygiene

When using do not eat or drink. Thorough skin-cleansing after handling the product.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Store locked up.

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.

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection. Wear face protection.

Skin protection



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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

NBR (Nitrile rubber)

material thickness

>0,11 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 $^{\circ}$ 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	yellow
Odour	characteristic
Melting point/freezing point	-21 °C
Boiling point or initial boiling point and boiling range	221 °C at 1.013 hPa
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	87 °C
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not determined

acc. to Regulation (EC) No. 1907/2006 (REACH)



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	Kinematic viscosity	1,15 ^{mm²} / _s at 20 °C
	Dynamic viscosity	1,3 mPa s at 20 °C
	Solubility(ies)	
	Water solubility	not determined
	Partition coefficient	
	Partition coefficient n-octanol/water (log value):	3,28 (Lit.)
	Vapour pressure	10 hPa at 20 °C
	Density and/or relative density	
	Density	1,13 ^g / _{cm³}
	Relative vapour density	4,65 (air = 1)
	Particle characteristics	not relevant (liquid)
	Other safety parameters	
	Oxidising properties	none
9.2	Other information	
	Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
	Other safety characteristics:	There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated

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

Material reacts vigorously with water emitting flammable gases, **Violent reaction with:** Alcohols, Amines, Chlorates, Nitrate, Oxidisers, Acids, Water, Alkalines

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

acc. to Regulation (EC) No. 1907/2006 (REACH)



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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Toxic if swallowed.

Acute toxicity

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	87 ^{mg} / _{kg}	mouse		TOXNET

Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

Respiratory or skin sensitisation

May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause an allergic skin reaction.

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

May produce an allergic reaction, cough, Dyspnoea

• If on skin

causes severe burns, causes poorly healing wounds, May produce an allergic reaction, pruritis, localised redness



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Other information

This information is based upon the present state of our knowledge.

- **11.2** Endocrine disrupting properties Does not contain an endocrine disruptor (EDC) in a concentration of $\ge 0,1\%$.
- 11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

12.2 Persistence and degradability

Data are not available.

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,28 (Lit.)
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12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

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

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (EDC) in a concentration of $\ge 0,1\%$.

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. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

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Properties of waste which render it hazardous

HP 6 acute toxicity

HP8 corrosive

HP 13 sensitising

HP 14 ecotoxic

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.

SEC	TION 14: Transport information	
14.1	UN number or ID number	
	ADRRID	UN 2922
	IMDG-Code	UN 2922
	ICAO-TI	UN 2922
14.2	UN proper shipping name	
	ADRRID	CORROSIVE LIQUID, TOXIC, N.O.S.
	IMDG-Code	CORROSIVE LIQUID, TOXIC, N.O.S.
	ICAO-TI	Corrosive liquid, toxic, n.o.s.
	Technical name	Phenyl isothiocyanate
14.3	Transport hazard class(es)	
	ADRRID	8 (6.1)
	IMDG-Code	8 (6.1)
	ICAO-TI	8 (6.1)
14.4	Packing group	
	ADRRID	II
	IMDG-Code	II
	ICAO-TI	II
14.5	Environmental hazards	hazardous to the aquatic environment
14.6	Special precautions for user	
	Provisions for dangerous goods (ADR) should be c	omplied within the premises.
14.7	Maritime transport in bulk according to IMO in	struments
	The cargo is not intended to be carried in bulk.	

14.8 Information for each of the UN Model Regulations



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Agreement concerning the International Carriage of Dangerous Goods by Road (ADR)Additional information		
Proper shipping name	CORROSIVE LIQUID, TOXIC, N.O.S.	
Particulars in the transport document	UN2922, CORROSIVE LIQUID, TOXIC, N.O.S., (Phenyl isothiocyanate), 8 (6.1), II, (E), environ- mentally hazardous	
Classification code	CT1	
Danger label(s)	8+6.1, "Fish and tree"	
Environmental hazards	Yes (hazardous to the aquatic environment)	
Special provisions (SP)	274, 802(ADN)	
Excepted quantities (EQ)	E2	
Limited quantities (LQ)	1 L	
Transport category (TC)	2	
Tunnel restriction code (TRC)	E	
Hazard identification No	86	
Emergency Action Code	2X	
Regulations concerning the International Carr information	iage of Dangerous Goods by Rail (RID)Additional	
Classification code	CT1	
Danger label(s)	8+6.1 Fish and tree	
Environmental hazards	Yes Hazardous to water	
Special provisions (SP)	274, 802(ADN)	
Excepted quantities (EQ)	E2	
Limited quantities (LQ)	1 L	
Transport category (TC)	2	
Hazard identification No	86	
International Maritime Dangerous Goods Code (IMDG) - Additional information		
Proper shipping name	CORROSIVE LIQUID, TOXIC, N.O.S.	
Particulars in the shipper's declaration	UN2922, CORROSIVE LIQUID, TOXIC, N.O.S., (Phenyl isothiocyanate), 8 (6.1), II, MARINE POL- LUTANT	
Marine pollutant	Yes (hazardous to the aquatic environment)	
Danger label(s)	8+6.1, "Fish and tree"	

acc. to Regulation (EC) No. 1907/2006 (REACH)



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Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-A, S-B
Stowage category	В
International Civil Aviation Organization (ICAC	D-IATA/DGR) - Additional information
Proper shipping name	Corrosive liquid, toxic, n.o.s.
Particulars in the shipper's declaration	UN2922, Corrosive liquid, toxic, n.o.s., (Phenyl iso- thiocyanate), 8 (6.1), II
Environmental hazards	Yes (hazardous to the aquatic environment)
Danger label(s)	8+6.1
Special provisions (SP)	A3, A4
Excepted quantities (EQ)	E2
Limited quantities (LQ)	0,5 L

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture 15.1 **Relevant provisions of the European Union (EU)**

Seveso Directive

2012/18/EU (Seveso III)				
Νο	Dangerous substance/hazard categories		(tonnes) for the ap- and upper-tier re- ments	Notes
H2	acute toxic (cat. 2 + cat. 3, inhal.)	50	200	41)

Notation

41) - Category 2, all exposure routes - category 3, inhalation exposure route

Deco-Paint Directive

VOC content	100 %
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Industrial Emissions Directive (IED)

VOC content	100 %
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Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

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Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Phenyl isothiocyanate	this product meets the criteria for classi- fication in accordance with Regulation No 1272/2008/EC		3

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
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed



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Country	Inventory	Status
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
CSCL-ENCS DSL ECSI IECSC ISHA-ENCS KECI NZIoC PICCS	Domestic Substances List EC Substance Inventory (I Inventory of Existing Chei Inventory of Existing and Korea Existing Chemicals New Zealand Inventory of	Chemical Substances (CSCL-ENCS) (DSL) EINECS, ELINCS, NLP) mical Substances Produced or Imported in China New Chemical Substances (ISHA-ENCS) Inventory f Chemicals nemicals and Chemical Substances (PICCS) nees cee Inventory

15.2 Chemical safety assessment

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

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of ≥ 0,1%.	yes
14.8	Special provisions (SP): A3	Special provisions (SP): A3, A4	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concern- ing the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identi- fier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Na- tions
ΙΑΤΑ	International Air Transport Association



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Abbr.	Descriptions of used abbreviations
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
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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
H301	Toxic if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

Disclaimer

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