

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



p-Nitrotoluene ROTI®CALIPURE 51-54 °C Melting point standard

article number: **9712**
Version: **5.0 en**
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Version: (4)

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

1.1 Product identifier

Identification of the substance	p-Nitrotoluene ROTI®CALIPURE 51-54 °C Melting point standard
Article number	9712
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
Index number in CLP Annex VI	609-006-00-3
EC number	202-808-0
CAS number	99-99-0

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

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 sheet: Department Health, Safety and Environment

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

1.4 Emergency telephone number

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.1O	Acute toxicity (oral)	3	Acute Tox. 3	H301
3.1D	Acute toxicity (dermal)	3	Acute Tox. 3	H311
3.1I	Acute toxicity (inhal.)	3	Acute Tox. 3	H331
3.9	Specific target organ toxicity - repeated exposure	2	STOT RE 2	H373
4.1C	Hazardous to the aquatic environment - chronic hazard	2	Aquatic Chronic 2	H411

For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Delayed or immediate effects can be expected after short or long-term exposure. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Danger

Pictograms

GHS06, GHS08,
GHS09



Hazard statements

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled
H373 May cause damage to organs (liver, testes) through prolonged or repeated exposure
H411 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
P311 Call a POISON CENTER/doctor

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled.

P280 Wear protective gloves/eye protection.
P302+P352 IF ON SKIN: Wash with plenty of water.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P311 Call a POISON CENTER/doctor.

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2.3 Other hazards

Endocrine disrupting properties

The substance has an endocrine disrupting potential.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	p-Nitrotoluene
Molecular formula	C ₇ H ₇ NO ₂
Molar mass	137,1 g/mol
CAS No	99-99-0
EC No	202-808-0
Index No	609-006-00-3

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	100 mg/kg 300 mg/kg >0,5 mg/l/4h	oral dermal inhalation: dust/ mist

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

Call a physician immediately. If breathing is irregular or stopped, administer artificial respiration.

Following skin contact

After contact with skin, wash immediately with plenty of water. In case of extensive skin contact serious poisoning possible. Call a physician in any case!

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Cardiac arrhythmias, Headache, Spasms, Dyspnoea, Methaemoglobinaemia, Blood pressure drop, Cyanosis (blue coloured blood)

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4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂)

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

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe dust.

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. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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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. Avoid dust formation. Clear contaminated areas thoroughly.

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. Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Store locked up.

Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted.

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.

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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

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: Dust formation. Particulate filter device (EN 143). P3 (filters at least 99,95 % of airborne particles, colour code: White).

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	solid
Form	crystalline
Colour	yellow
Odour	characteristic
Melting point/freezing point	44,5 °C (ECHA)
Boiling point or initial boiling point and boiling range	238,3 °C at 101 kPa (ECHA)
Flammability	this material is combustible, but will not ignite readily

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Lower and upper explosion limit	1,6 vol% (LEL)
Flash point	103 °C at 1.013 hPa (ECHA)
Auto-ignition temperature	450 °C (ECHA) (relative self-ignition temperature for solids)
Decomposition temperature	not relevant
pH (value)	not applicable
Kinematic viscosity	not relevant

Solubility(ies)

Water solubility 0,345 g/l at 20 °C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 2,37 (25 °C) (ECHA)

Vapour pressure 0,13 hPa at 20 °C

Density and/or relative density

Density 1,1 – 1,2 g/cm³ at 20 °C

Relative vapour density Information on this property is not available.

Particle characteristics No data available.

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:

Temperature class (EU, acc. to ATEX) T2
Maximum permissible surface temperature on the equipment: 300°C

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

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

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10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Strong alkali, Strong oxidiser, Ammonia (NH₃), Strong acid, Reducing agent, Sulphur trioxide,
=> Explosive properties

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

plastic and rubber

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Toxic if swallowed. Toxic in contact with skin. Toxic if inhaled.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
dermal	LD50	>16.000 mg/kg	rabbit		TOXNET
oral	LD50	>2.250 mg/kg	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

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

May cause damage to organs (liver, testes) through prolonged or repeated exposure.

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Hazard category	Target organ	Exposure route
2	liver	if exposed
2	testes	if exposed

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

Data are not available.

• If in eyes

causes slight to moderate irritation

• If inhaled

irritant effects, headache

• If on skin

causes slight to moderate irritation, risk of absorption via the skin

• Other information

Other adverse effects, Cardiac arrhythmias, Dyspnoea, Blood pressure drop, Spasms, Methaemoglobinemia, Cyanosis (blue coloured blood)

11.2 Endocrine disrupting properties

This substance is known as an "endocrine disruptor".

Endocrine disrupting chemicals (EDC)				
Name of substance	CAS No	Combined category	Human health category	Wildlife category
p-Nitrotoluene	99-99-0	CAT1	CAT1	CAT3

Legend

CAT1 Category 1 - evidence of endocrine disruption in at least one species using intact animals
CAT3 Category 3 - no evidence of endocrine disruption or no data available

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
EC50	4,2 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	22 mg/l	algae	ECHA	96 h

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Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	5 mg/l	microorganisms	ECHA	15 min

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,633 mg/mg

Theoretical Oxygen Demand (with nitrification): 2,1 mg/mg

Theoretical Carbon Dioxide: 2,246 mg/mg

Process of degradability

Process	Degradation rate	Time
DOC removal	94 %	15 d
oxygen depletion	0,8 %	14 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	2,37 (25 °C) (ECHA)
BCF	39,26

12.4 Mobility in soil

Henry's law constant	2,38 Pa m ³ /mol at 25 °C (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

This substance is known as an "endocrine disruptor".

Endocrine disrupting chemicals (EDC)

Name of substance	CAS No	Combined category	Human health category	Wildlife category
p-Nitrotoluene	99-99-0	CAT1	CAT1	CAT3

Legend

CAT1 Category 1 - evidence of endocrine disruption in at least one species using intact animals
CAT3 Category 3 - no evidence of endocrine disruption or no data available

12.7 Other adverse effects

Data are not available.

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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.

Properties of waste which render it hazardous

HP 5 specific target organ toxicity (STOT)/aspiration toxicity

HP 6 acute toxicity

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.

SECTION 14: Transport information

14.1 UN number or ID number

ADR UN 3446

IMDG-Code UN 3446

ICAO-TI UN 3446

14.2 UN proper shipping name

ADR NITROTOLUENES, SOLID

IMDG-Code NITROTOLUENES, SOLID

ICAO-TI Nitrotoluenes, solid

14.3 Transport hazard class(es)

ADR 6.1

IMDG-Code 6.1

ICAO-TI 6.1

14.4 Packing group

ADR II

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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 complied within the premises.

14.7 Maritime 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

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) Additional information

Proper shipping name	NITROTOLUENES, SOLID
Particulars in the transport document	UN3446, NITROTOLUENES, SOLID, 6.1, II, (D/E), environmentally hazardous
Classification code	T2
Danger label(s)	6.1, "Fish and tree"
	
Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	802(ADN)
Excepted quantities (EQ)	E4
Limited quantities (LQ)	500 g
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	60

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	NITROTOLUENES, SOLID
Particulars in the shipper's declaration	UN3446, NITROTOLUENES, SOLID, 6.1, II, MARINE POLLUTANT
Marine pollutant	yes (hazardous to the aquatic environment)
Danger label(s)	6.1, "Fish and tree"
	
Special provisions (SP)	-
Excepted quantities (EQ)	E4
Limited quantities (LQ)	500 g
EmS	F-A, S-A
Stowage category	A

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

Proper shipping name	Nitrotoluenes, solid
Particulars in the shipper's declaration	UN3446, Nitrotoluenes, solid, 6.1, II
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	6.1



Excepted quantities (EQ)	E4
Limited quantities (LQ)	1 kg

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

Seveso Directive

2012/18/EU (Seveso III)

No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		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 %
VOC content	1.200 g/l

Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.200 g/l

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

not listed

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

not listed

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Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
p-Nitrotoluene	Substances and preparations, or the breakdown products of such, which have been proved to possess carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrine-related functions in or via the aquatic environment		a)	

Legend

a) Indicative list of the main pollutants

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

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
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

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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
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.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3	Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.		yes
15.1	VOC content: 100 % 1.200 g/l	VOC content: 100 %	yes
15.1		VOC content: 1.200 g/l	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 concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
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
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier 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
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control

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Abbr.	Descriptions of used abbreviations
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
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
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
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). 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.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H373	May cause damage to organs (liver, testes) through prolonged or repeated exposure.
H411	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.