

# Safety data sheet

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



**o-Nitrotoluene ≥99%, for synthesis**

article number: **0961**

Version: **3.0 en**

Replaces version of: 2022-06-30

Version: (2)

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Revision: 2022-06-30

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

### 1.1 Product identifier

Identification of the substance	<b>o-Nitrotoluene ≥99%, for synthesis</b>
Article number	0961
EC number	201-853-3
CAS number	88-72-2

### 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 products which come into contact with foodstuffs. Do not use for private purposes (household).

### 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

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

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.5	Germ cell mutagenicity	1B	Muta. 1B	H340
3.6	Carcinogenicity	1B	Carc. 1B	H350

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.7	Reproductive toxicity	2	Repr. 2	H361f
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

Spillage and fire water can cause pollution of watercourses.

## 2.2 Label elements

### Labelling

#### Signal word

**Danger**

#### Pictograms

GHS07, GHS08,  
GHS09



#### Hazard statements

H302	Harmful if swallowed
H340	May cause genetic defects
H350	May cause cancer
H361f	Suspected of damaging fertility
H411	Toxic to aquatic life with long lasting effects

#### Precautionary statements

##### Precautionary statements - prevention

P201	Obtain special instructions before use
P273	Avoid release to the environment
P280	Wear protective gloves/eye protection

##### Precautionary statements - response

P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell
P308+P313	IF exposed or concerned: Get medical advice/attention

For professional users only

## 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.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	o-Nitrotoluene
Molecular formula	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>
Molar mass	137,1 g/mol
CAS No	88-72-2
EC No	201-853-3

#### Substance, Specific Conc. Limits, M-factors, ATE

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	891 mg/kg	oral

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

#### Following inhalation

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

#### Following skin contact

Rinse skin with water/shower.

#### 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 with water (only if the person is conscious). In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible). Call a doctor.

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

Following inhalation: Cough, pain, choking, and breathing difficulties,

Following skin contact: Irritant effects,

After eye contact: Irritant,

Following ingestion: Nausea, Vomiting

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

none

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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 (CO<sub>2</sub>)

#### 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<sub>x</sub>), 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. 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.

## 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.

### 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.

### 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.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid exposure.

#### Measures to protect the environment

Avoid release to the environment.

#### Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

### 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:

#### 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.

##### Skin protection



##### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. 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

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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)

- **material thickness**

0,5 mm

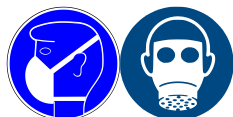
- **breakthrough times of the glove material**

>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  $> 65\text{ }^{\circ}\text{C}$ , 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	$-9,3\text{ }^{\circ}\text{C}$ (ECHA)
Boiling point or initial boiling point and boiling range	$222\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	1,47 vol% (LEL) - 8,8 vol% (UEL)
Flash point	$95\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Auto-ignition temperature	$420\text{ }^{\circ}\text{C}$ (ECHA) (auto-ignition temperature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	6 – 8
Kinematic viscosity	not determined
<u>Solubility(ies)</u>	
Water solubility	$0,437\text{ g/l}$ at $20\text{ }^{\circ}\text{C}$ (ECHA)

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### Partition coefficient

Partition coefficient n-octanol/water (log value): 2,3 (ECHA)

Vapour pressure

0,16 hPa at 20 °C

### Density and/or relative density

Density

1,16 g/cm<sup>3</sup> at 20 °C (ECHA)

Relative vapour density

information on this property is not available

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**

**Violent reaction with:** strong oxidiser, Ammonia (NH<sub>3</sub>), Sodium, Strong acid, Sodium and potassium hydroxide, Explosive properties,  
=> Bases, Reducing agents, Sulphuric acid, Sulphur trioxide

### **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.

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Classification acc. to GHS

##### Acute toxicity

Harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	891 mg/kg	rat		TOXNET

##### 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

May cause genetic defects.

##### Carcinogenicity

May cause cancer.

##### Reproductive toxicity

Suspected of damaging fertility.

##### 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

vomiting, nausea

##### • If in eyes

slightly irritant but not relevant for classification

##### • If inhaled

cough, pain, choking, and breathing difficulties

##### • If on skin

slightly irritant but not relevant for classification

##### • Other information

Other adverse effects: Liver and kidney damage, Cardiovascular system, Cardiac arrhythmias, Head-ache, Blood pressure drop, Spasms, Cyanosis (blue coloured blood)



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## 11.2 Endocrine disrupting properties

Not listed.

## 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	5,4 mg/l	aquatic invertebrates	ECHA	48 h
LC50	8,8 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	22 mg/l	algae	ECHA	72 h

### Biodegradation

Data are not available.

### 12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,042 mg/mg  
Theoretical Oxygen Demand: 1,633 mg/mg  
Theoretical Carbon Dioxide: 2,246 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	2,3 (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

Not listed.

### 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.

### 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. Waste catalogue ordinance (Germany).

### 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.

## SECTION 14: Transport information

### 14.1 UN number or ID number

ADRRID	UN 1664
IMDG-Code	UN 1664
ICAO-TI	UN 1664

### 14.2 UN proper shipping name

ADRRID	NITROTOLUENES, LIQUID
IMDG-Code	NITROTOLUENES, LIQUID
ICAO-TI	Nitrotoluenes, liquid

### 14.3 Transport hazard class(es)

ADRRID	6.1
IMDG-Code	6.1
ICAO-TI	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 complied within the premises.

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### **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**

#### **Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information**

Proper shipping name	NITROTOLUENES, LIQUID
Particulars in the transport document	UN1664, NITROTOLUENES, LIQUID, 6.1, II, (D/E), environmentally hazardous
Classification code	T1
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)	100 ml
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	60
<b>Emergency Action Code</b>	<b>2X</b>

#### **Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information**

<b>Classification code</b>	T1
<b>Danger label(s)</b>	6.1 Fish and tree
	
<b>Environmental hazards</b>	Yes Hazardous to water
<b>Special provisions (SP)</b>	802(ADN)
<b>Excepted quantities (EQ)</b>	E4
<b>Limited quantities (LQ)</b>	100 ml
<b>Transport category (TC)</b>	2
<b>Hazard identification No</b>	60

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

Proper shipping name	NITROTOLUENES, LIQUID
Particulars in the shipper's declaration	UN1664, NITROTOLUENES, LIQUID, 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)	100 mL
EmS	F-A, S-A
Stowage category	A

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

Proper shipping name	Nitrotoluenes, liquid
Particulars in the shipper's declaration	UN1664, Nitrotoluenes, liquid, 6.1, II
Environmental hazards	YES (hazardous to the aquatic environment)
Danger label(s)	6.1
Excepted quantities (EQ)	E4
Limited quantities (LQ)	1 L

## 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)

##### 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
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200                      500	57)

##### Notation

57) Hazardous to the Aquatic Environment in category Chronic 2

##### Deco-Paint Directive

VOC content	100 % 1.160 g/l
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## Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.160 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

## Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
o-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

## 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
o-Nitrotoluene	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
o-Nitrotoluene	carcinogenic		28

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### Dangerous substances with restrictions (GB REACH, Annex 17)

Name of substance	Name acc. to inventory	CAS No	No
o-Nitrotoluene	germ cell mutagenic (mutagenic)		29

### 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

#### 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
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)

Alignment to regulation:

Restructuring: section 9, section 14

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.2		Precautionary statements - prevention: change in the listing (table)	yes

## Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
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
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
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
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 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
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

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Abbr.	Descriptions of used abbreviations
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
UEL	Upper explosion limit (UEL)
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
H302	Harmful if swallowed.
H340	May cause genetic defects.
H350	May cause cancer.
H361f	Suspected of damaging fertility.
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.