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



3-Nitroaniline 99%, for synthesis

article number: 9867 date of compilation: 2016-07-29 Version: 3.0 en Revision: 2024-03-02

Replaces version of: 2022-01-12

Version: (2)

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

Product identifier 1.1

Identification of the substance **3-Nitroaniline** 99%, for synthesis

Article number 9867

Registration number (REACH) It is not required to list the identified uses be-

cause the substance is not subject to registration

according to REACH (< 1 t/a).

Index number in CLP Annex VI 612-012-00-9 EC number 202-729-1 CAS number 99-09-2

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

sicherheit@carlroth.de

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 Department Health, Safety and Environment

sheet:

1.4

e-mail (competent person): **Emergency telephone number**

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	https:// www.poisons.ie/

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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
3.10	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	3	Aquatic Chronic 3	H412

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





Hazard statements

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

H373 May cause damage to organs through prolonged or repeated exposure

H412 Harmful to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P280 Wear protective clothing/eye protection/face protection

Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor

P302+P352 IF ON SKIN: Wash with plenty of water

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing

P312 Call a POISON CENTRE/doctor if you feel unwell

Labelling of packages where the contents do not exceed 125 ml

Signal word: Danger

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Symbol(s)



H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled. Harmful to aquatic life with long lasting effects.

P280 Wear protective clothing/eye protection/face protection. P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.

P302+P352 IF ON SKIN: Wash with plenty of water.

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTRE/doctor if you feel unwell. P304+P340

P312

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**

3-Nitroaniline Name of substance Molecular formula $C_6H_6N_2O_2$ Molar mass 138,1 ^g/_{mol} CAS No 99-09-2 EC No 202-729-1 612-012-00-9 Index No

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

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	100 ^{mg} / _{kg} 300 ^{mg} / _{kg} >0,5 ^{mg} / _I /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.

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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

Symptoms and effects are not known to date.

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, alcohol resistant 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 (NOx), 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

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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.

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 prevent fire as well as aerosol and dust generation

Removal of dust deposits.

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

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. 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)

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Coun	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
IE	dusts, non-specific		OELV	10			i	S.I. No. 619 of 2001
IE	dusts, non-specific		OELV	4			r	S.I. No. 619 of 2001

Notation

Ceiling value is a limit value above which exposure should not occur Ceiling-C

Inhalable fraction Respirable fraction

Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified) STEL

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8

hours time-weighted average (unless otherwise specified)

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. 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.

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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

Colour yellow-orange
Odour characteristic
Melting point/freezing point 109 – 112 °C

Boiling point or initial boiling point and boiling

range

306 °C

Flammability this material is combustible, but will not ignite

readily

Lower and upper explosion limit not determined

Flash point 196 °C

Auto-ignition temperature not determined

Decomposition temperature 247 °C at 1.013 hPa

pH (value) not applicable Kinematic viscosity not relevant

Solubility(ies)

Water solubility 1,25 g/l at 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value): 1,37 (TOXNET)

Vapour pressure 1 hPa at 104 °C

Density and/or relative density

Density $0.9 \, \mathrm{g/_{cm^3}}$

Relative vapour density Information on this property is not available.

Particle characteristics No data available.

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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) T1

Maximum permissible surface temperature on

the equipment: 450°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.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Alkali metals, Magnesium, Organic substances, Nitric acid, Sulphuric acid, Water

10.4 Conditions to avoid

Keep away from heat. Humidity. Decompostion takes place from temperatures above: $247 \, ^{\circ}\text{C}$ at $1.013 \, \text{hPa}$.

10.5 Incompatible materials

There is no additional information.

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.

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.

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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 through prolonged or repeated exposure.

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

Data are not available.

If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

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

11.2 Endocrine disrupting properties

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

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,158 mg / $_{mg}$ Theoretical Oxygen Demand (with nitrification): 1,651 mg / $_{mg}$ Theoretical Carbon Dioxide: 1,912 mg / $_{mg}$

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,37 (TOXNET)

12.4 Mobility in soil

Data are not available.

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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. 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

ADRRID UN 1661 IMDG-Code UN 1661 ICAO-TI UN 1661

14.2 UN proper shipping name

ADRRID NITROANILINES
IMDG-Code NITROANILINES
ICAO-TI Nitroanilines

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	14.3	Transport hazard class(es)
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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 non-environmentally hazardous acc. to the dan-

gerous goods regulations

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.

I.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 NITROANILINES

Particulars in the transport document UN1661, NITROANILINES, 6.1, II, (D/E)

Classification code T2
Danger label(s) 6.1



Special provisions (SP) 279, 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

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

Classification code T2

Danger label(s) 6.1



Special provisions (SP) 279, 802(ADN)

Excepted quantities (EQ) E4

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Limited quantities (LQ)500 gTransport category (TC)2Hazard identification No60

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name NITROANILINES

Particulars in the shipper's declaration UN1661, NITROANILINES, 6.1, II

Marine pollutant Danger label(s) 6.1



Special provisions (SP) 279

Excepted quantities (EQ) E4

Limited quantities (LQ) 500 g

EmS F-A, S-A

Stowage category A

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

Proper shipping name Nitroanilines

Particulars in the shipper's declaration UN1661, Nitroanilines, 6.1, II

Danger label(s) 6.1



Special provisions (SP) A113
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.

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Seveso Directive

2012/18/EU (Seveso III)						
No	Dangerous substance/hazard categories	Qualifying quantity plication of lower quirer		Notes		
H2	acute toxic (cat. 2 + cat. 3, inhal.)	50	200	41)		

Notation

Deco-Paint Directive

VOC content	0 %

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

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
3-Nitroaniline	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 endocrinerelated functions in or via the aquatic environment		a)	

Legend

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

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⁻ Category 2, all exposure routes - category 3, inhalation exposure route

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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 List of Existing and New Chemical Substances (CSCL-ENCS) CSCL-ENCS

Domestic Substances List (DSL)

DSL ECSI IECSC

EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China National Inventory of Chemical Substances
Korea Existing Chemicals Inventory
National Chemical Inventory
New Zealand Inventory of Chemicals
Philippine Inventory of Chemicals and Chemical Substances (PICCS) INSO

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- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8		Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
14.8		Classification code: T2	yes
14.8		Danger label(s): 6.1	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Special provisions (SP): 279, 802(ADN)	yes
14.8		Excepted quantities (EQ): E4	yes
14.8		Limited quantities (LQ): 500 g	yes
14.8		Transport category (TC): 2	yes
14.8		Hazard identification No: 60	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)	
Ceiling-C	Ceiling value	
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures	
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 ident fier of substances commercially available within the EU (European Union)	
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	

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Abbr.	Descriptions of used abbreviations
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
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)
S.I. No. 619 of 2001	Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
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). 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.	
H311	Toxic in contact with skin.	
H331	Toxic if inhaled.	
H373	May cause damage to organs through prolonged or repeated exposure.	
H412	Harmful 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.

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