

Safety data sheet

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



3-Chloroaniline ≥98 %, for synthesis

article number: **1C3E**
Version: **3.0 en**
Replaces version of: 2022-05-06
Version: (2)

date of compilation: 2020-05-26
Revision: 2024-03-03

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

1.1 Product identifier

Identification of the substance	3-Chloroaniline ≥98 %, for synthesis
Article number	1C3E
Index No (GB CLP)	612-010-00-8
EC number	203-581-0
CAS number	108-42-9

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). 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

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

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Classification acc. to GHS

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
4.1A	Hazardous to the aquatic environment - acute hazard	1	Aquatic Acute 1	H400
4.1C	Hazardous to the aquatic environment - chronic hazard	1	Aquatic Chronic 1	H410

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

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 through prolonged or repeated exposure
H410 Very toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P260 Do not breathe mist/vapours/spray
P273 Avoid release to the environment
P280 Wear protective gloves/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 soap and water
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing

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2.3 Other hazards

Results of PBT and vPvB assessment

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

Endocrine disrupting properties

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

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	3-Chloroaniline
Molecular formula	C ₆ H ₆ ClN
Molar mass	127,6 g/mol
CAS No	108-42-9
EC No	203-581-0
Index No (GB CLP)	612-010-00-8

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	100 mg/kg 300 mg/kg 3 mg/l/4h	oral dermal inhalation: vapour

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.

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

Irritant effects, Has degreasing effect on the skin, Nausea, Vomiting, Headache, Cough, Dyspnoea, Spasms, Blood pressure drop, Cardiac arrhythmias, Methaemoglobinaemia, 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 spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

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), Hydrogen chloride (HCl)

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 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.

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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. 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. May cause decomposition by long-term light influence.

Incompatible substances or mixtures

Observe hints for combined storage.

Protect against external exposure, such as

UV-radiation/sunlight, contact with air/oxygen

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.

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	0,367 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,208 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

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Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,003 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	9,9 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,753 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,753 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,331 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

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

• type of material

Butyl caoutchouc (butyl rubber)

• material thickness

$\geq 0,5$ mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• Splash protection - Protective gloves

• type of material: NR: natural rubber, latex

• material thickness: 0,65 mm

• breakthrough times of the glove material: >30 minutes (permeation: level 2)

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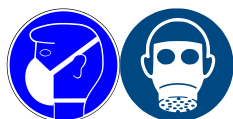
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• other protection measures

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	colourless - light yellow
Odour	characteristic
Melting point/freezing point	$-10,28\text{ }^{\circ}\text{C}$ (ECHA)
Boiling point or initial boiling point and boiling range	$168,8\text{ }^{\circ}\text{C}$ at 960 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	$110\text{ }^{\circ}\text{C}$ at 960 hPa (ECHA)
Auto-ignition temperature	$>500\text{ }^{\circ}\text{C}$
Decomposition temperature	$>190\text{ }^{\circ}\text{C}$
pH (value)	not determined (neutral)
Kinematic viscosity	$16,37\text{ mm}^2/\text{s}$ at $30\text{ }^{\circ}\text{C}$
Dynamic viscosity	$19,41\text{ mPa s}$ at $30\text{ }^{\circ}\text{C}$
<u>Solubility(ies)</u>	
Water solubility	20 g/l at $30\text{ }^{\circ}\text{C}$ (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	this information is not available
Soil organic carbon/water (log KOC)	2,398 (ECHA)
Vapour pressure	$8,799\text{ Pa}$ at $25\text{ }^{\circ}\text{C}$
<u>Density and/or relative density</u>	

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Density	1,186 g/cm ³ at 30 °C (ECHA)
Relative vapour density	Information on this property is not available.
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none
9.2 Other information	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	
Surface tension	45,3 mN/m (25 °C) (ECHA)

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, Carboxylic acid anhydride, Acetic anhydride, Acids, Acid chlorides, inorganic

10.4 Conditions to avoid

UV-radiation/sunlight. Keep away from heat. Decomposition takes place from temperatures above: >190 °C.

10.5 Incompatible materials

different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

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.

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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 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

vomiting, nausea

• If in eyes

causes slight to moderate irritation

• If inhaled

headache, cough, Dyspnoea

• If on skin

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation)

• Other information

Other adverse effects: Liver and kidney damage, Cardiac arrhythmias, Blood pressure drop, Spasms, Methaemoglobinaemia, Cyanosis (blue coloured blood)

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.

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SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,63 mg/mg

Theoretical Oxygen Demand (with nitrification): 2,132 mg/mg

Theoretical Carbon Dioxide: 2,07 mg/mg

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Henry's law constant	0,143 Pa m ³ /mol at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	2,398 (ECHA)

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

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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
Emergency Action Code	2X

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

Classification code	T1
Danger label(s)	6.1, "Fish and tree"



Environmental hazards	Yes Hazardous to water
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Special provisions (SP)	802(ADN)
Excepted quantities (EQ)	E4
Limited quantities (LQ)	100 ml
Transport category (TC)	2
Hazard identification No	60

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	CHLOROANILINES, LIQUID
Particulars in the shipper's declaration	UN2019, CHLOROANILINES, 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

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

Proper shipping name	Chloroanilines, liquid
Particulars in the shipper's declaration	UN2019, Chloroanilines, 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
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	0 %
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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-Chloroaniline	Organohalogen compounds and substances which may form such compounds in the aquatic environment		a)	

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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
3-Chloroaniline	this product meets the criteria for classification 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
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)

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Country	Inventory	Status
VN	NCI	substance is listed

Legend

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

15.2 Chemical safety assessment

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

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	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
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
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)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GB CLP	The Chemicals (Health and Safety) and Genetically Modified Organisms (Contained Use) (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/720 (as amended)
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

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Abbr.	Descriptions of used abbreviations
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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations 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.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.
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.