

## Acetonitrile for HPLC gradient grade

Version number: GHS 2.0  
Replaces version of: 2024-07-16 (GHS 1)

Revision: 2025-05-16

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

#### 1.1 Product identifier

**Identification of the substance** Acetonitrile for HPLC gradient grade  
**CAS number** 75-05-8  
**Article number** LC-5413

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

**Relevant identified uses** General use

#### 1.3 Details of the supplier of the safety data sheet

NeoFroxx GmbH  
Marie-Curie-Str. 3  
D-64683 Einhausen  
Germany

Telephone: +49 (6251) 989 24 - 0  
e-mail: info@neofroxx.com  
Website: neofroxx.com

**e-mail (competent person)** info@neofroxx.com (neoFroxx GmbH)

#### 1.4 Emergency telephone number

Poison centre			
Country	Name	Postal code/city	Telephone
United Kingdom	National Poisons Information Service		111

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and category	Hazard statement
2.6	flammable liquid	2	Flam. Liq. 2	H225
3.1O	acute toxicity (oral)	4	Acute Tox. 4	H302
3.1D	acute toxicity (dermal)	4	Acute Tox. 4	H312
3.1I	acute toxicity (inhal.)	4	Acute Tox. 4	H332
3.3	serious eye damage/eye irritation	2	Eye Irrit. 2	H319

For full text of abbreviations: see SECTION 16.

#### The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

#### 2.2 Label elements

##### Labelling

- Signal word danger

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### - Pictograms

GHS02, GHS07



### - Hazard statements

H225 Highly flammable liquid and vapour.  
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.  
H319 Causes serious eye irritation.

### - Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P233 Keep container tightly closed.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.  
P312 Call a POISON CENTRE/doctor if you feel unwell.  
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher to extinguish.  
P403+P235 Store in a well-ventilated place. Keep cool.  
P501 Dispose of contents/container to industrial combustion plant.

## 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** Acetonitrile for HPLC gradient grade

#### Identifiers

CAS No 75-05-8  
EC No 200-835-2  
Index No 608-001-00-3  
(GB CLP)

**Purity** >99 %

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	469 mg/kg 1,111 mg/kg 6.022 mg/l/4h	oral dermal inhalation: vapour

**Molecular formula** C<sub>2</sub>H<sub>3</sub>N

**Molar mass** 41.05 g/mol

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### SECTION 4: First aid measures

#### 4.1 Description of first aid measures

##### General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

##### Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. Provide fresh air.

##### Following skin contact

Wash with plenty of soap and water.

##### Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

##### Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

#### 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

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

Water jet

#### 5.2 Special hazards arising from the substance or mixture

In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

##### Hazardous combustion products

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. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

### SECTION 6: Accidental release measures

#### 6.1 Personal precautions, protective equipment and emergency procedures

##### For non-emergency personnel

Remove persons to safety.

##### For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

#### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

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### 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

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

#### Appropriate containment techniques

Use of adsorbent materials.

#### 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

#### Recommendations

#### - Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation. Avoidance of ignition sources. Keep away from sources of ignition - No smoking. Take precautionary measures against static discharge. Use only in well-ventilated areas. Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools.

#### - Specific notes/details

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

#### Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Managing of associated risks

#### - Explosive atmospheres

Keep container tightly closed and in a well-ventilated place. Use local and general ventilation. Keep cool. Protect from sunlight.

#### - Flammability hazards

Keep away from sources of ignition - No smoking. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge. Protect from sunlight.

#### - 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. Ground/bond container and receiving equipment.

#### - Packaging compatibilities

Only packagings which are approved (e.g. acc. to ADR) may be used.

### 7.3 Specific end use(s)

See section 16 for a general overview.

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### SECTION 8: Exposure controls/personal protection

#### 8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)											
Country	Name of agent	CAS No	Identifier	TWA [ppm]	TWA [mg/m <sup>3</sup> ]	STEL [ppm]	STEL [mg/m <sup>3</sup> ]	Ceiling-C [ppm]	Ceiling-C [mg/m <sup>3</sup> ]	Notation	Source
EU	acetonitrile	75-05-8	IOELV	40	70					H	2006/15/EC
GB	acetonitrile	75-05-8	WEL	40	68	60	102				EH40/2005

#### Notation

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

H absorbed through the skin

STEL 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)

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)

#### Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	68 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	68 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	68 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - local effects
DNEL	68 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	acute - local effects
DNEL	32.2 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

#### Environmental values

Relevant PNECs and other threshold levels				
Endpoint	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	10 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	1 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	32 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	7.53 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	2.41 mg/kg	terrestrial organisms	soil	short-term (single instance)

#### 8.2 Exposure controls

##### Appropriate engineering controls

General ventilation.

##### Individual protection measures (personal protective equipment)

##### Eye/face protection

Wear eye/face 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. In the case of wanting to use the gloves again, clean them before taking off and air them well. 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.

- Type of material

NBR: acrylonitrile-butadiene rubber

- Material thickness

min. 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. Wash hands thoroughly after handling.

### Respiratory protection

P2 (filters at least 94 % of airborne particles, colour code: White).

### Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

<b>Physical state</b>	liquid
<b>Colour</b>	colourless
<b>Odour</b>	like ether
<b>Odour threshold</b>	39.8 ppm
<b>Melting point/freezing point</b>	-45.7 °C
<b>Boiling point or initial boiling point and boiling range</b>	81.6 °C at 1,013 hPa
<b>Flammability</b>	flammable liquid in accordance with GHS criteria
<b>Lower and upper explosion limit</b>	not determined
<b>Flash point</b>	12.8 °C
<b>Auto-ignition temperature</b>	524 °C (ECHA)
<b>Decomposition temperature</b>	not relevant
<b>pH (value)</b>	not determined
<b>Kinematic viscosity</b>	not determined

### Solubility(ies)

Water solubility	1,000,000 mg/l at 25 °C
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### Partition coefficient

Partition coefficient n-octanol/water (log value)	this information is not available
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Vapour pressure	94.51 hPa at 20 °C
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### Density and/or relative density

Density	0.78 g/cm <sup>3</sup> at 20 °C
Relative vapour density	information on this property is not available

Particle characteristics	not relevant (liquid)
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### 9.2 Other information

<b>Information with regard to physical hazard classes</b>	there is no additional information
<b>Other safety characteristics</b>	there is no additional information

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials". It's a reactive substance. The mixture contains reactive substance(s). Risk of ignition.

If heated:

Risk of ignition

### 10.2 Chemical stability

See below "Conditions to avoid".

### 10.3 Possibility of hazardous reactions

No known hazardous reactions.

### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

#### Hints to prevent fire or explosion

Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools. Take precautionary measures against static discharge.

### 10.5 Incompatible materials

Oxidisers

### 10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. 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. Harmful in contact with skin. Harmful if inhaled.

##### - Acute toxicity estimate (ATE)

Oral 469 mg/kg  
Dermal 1,111 mg/kg  
Inhalation: vapour 6.022 mg/l/4h

Acute toxicity			
Exposure route	Endpoint	Value	Species
oral	LD50	469 mg/kg	mouse
dermal	LD50	>2,000 mg/kg	rabbit
inhalation: vapour	LC50	6.022 mg/l/4h	mouse

##### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

##### Serious eye damage/eye irritation

Causes serious eye irritation.

##### 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

Shall not be classified as a specific target organ toxicant (repeated exposure).

##### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

#### 11.2 Information on other hazards

There is no additional information.

### SECTION 12: Ecological information

#### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

#### 12.2 Persistence and degradability

##### Biodegradation

The substance is readily biodegradable.

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Process of degradability		
Process	Degradation rate	Time
carbon dioxide generation	70 %	21 d

### 12.3 Bioaccumulative potential

Data are not available.

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

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

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (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

#### Waste treatment-relevant information

Solvent reclamation/regeneration.

#### 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. Completely emptied packages can be recycled. Handle contaminated packages in the same way as the substance itself.

#### Remarks

Please consider the relevant national or regional provisions. Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities.

## SECTION 14: Transport information

### 14.1 UN number or ID number

ADR/RID	UN 1648
IMDG-Code	UN 1648
ICAO-TI	UN 1648

### 14.2 UN proper shipping name

ADR/RID	ACETONITRILE
IMDG-Code	ACETONITRILE
ICAO-TI	Acetonitrile

### 14.3 Transport hazard class(es)

ADR/RID	3
IMDG-Code	3
ICAO-TI	3

### 14.4 Packing group

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<b>ADR/RID</b>	II
<b>IMDG-Code</b>	II
<b>ICAO-TI</b>	II
<b>14.5 Environmental hazards</b>	non-environmentally hazardous acc. to the dangerous goods regulations
<b>14.6 Special precautions for user</b>	Provisions for dangerous goods (ADR) should be complied within the premises.
<b>14.7 Maritime transport in bulk according to IMO instruments</b>	The cargo is not intended to be carried in bulk.

### Information for each of the UN Model Regulations


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

Classification code	F1
Danger label(s)	3
	
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	33
Emergency Action Code	2YE

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

Classification code	F1
Danger label(s)	3
	
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Hazard identification No	33

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

Marine pollutant	-
Danger label(s)	3
	
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

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EmS F-E, S-D

Stowage category B

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

Danger label(s) 3



Excepted quantities (EQ) E2

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)

##### Deco-Paint Directive

VOC content	100 %
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##### Industrial Emissions Directive (IED)

VOC content	100 %
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##### Water Framework Directive (WFD)

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
Acetonitrile for HPLC gradient grade	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
Acetonitrile for HPLC gradient grade	flammable / pyrophoric		40

##### Storage of hazardous substances in non-stationary containers (TRGS 510) (Germany)

Storage class (LGK) 3 (flammable or desensitizing explosive liquids)

##### National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed

##### Legend

REACH Reg. REACH registered substances

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### 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
3.1		Purity: >99 %	yes
3.1		Purity: change in the listing (table)	yes
11.1		- Acute toxicity estimate (ATE): change in the listing (table)	yes
11.1		Acute toxicity: change in the listing (table)	yes
15.1		Storage of hazardous substances in non-stationary containers (TRGS 510) (Germany)	yes
15.1		Storage class (LGK): 3 (flammable or desensitizing explosive liquids)	yes
16		Abbreviations and acronyms: change in the listing (table)	yes

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
2006/15/EC	Commission Directive establishing a second list of indicative occupational exposure limit values in implementation of Council Directive 98/24/EC and amending Directives 91/322/EEC and 2000/39/EC
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)
Ceiling-C	Ceiling value
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
EH40/2005	EH40/2005 Workplace exposure limits ( <a href="http://www.nationalarchives.gov.uk/doc/open-government-licence/">http://www.nationalarchives.gov.uk/doc/open-government-licence/</a> )
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
IATA	International Air Transport Association

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Abbr.	Descriptions of used abbreviations
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
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
IOELV	Indicative occupational exposure limit value
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
LGK	Lagerklasse (storage class according to TRGS 510, Germany)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	Parts per million
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)
STEL	Short-term exposure limit
TRGS	Technische Regeln für Gefahrstoffe (technical rules for hazardous substances, Germany)
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

### 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
H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

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### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product. The information is intended to give you guidelines for the safe handling of the product mentioned in this safety data sheet during storage, processing, transport and disposal. The information is not transferable to other products. Insofar as the product is mixed, blended or processed with other materials or is subjected to processing, the information in this safety data sheet cannot be transferred to the new material produced in this way, unless expressly stated otherwise.