

Safety data sheet Safety data sheet

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



4-Nitrobenzyl chloride \geq 98%, for synthesis

article number: **5697**
Version: **2.0 en**
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Version: (1)

date of compilation: 2021-06-29
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Identification of the substance	4-Nitrobenzyl chloride \geq 98%, for synthesis
Article number	5697
EC number	202-822-7
CAS number	100-14-1

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for squirting or spraying. Do not use for products which come into direct contact with the skin. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

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
3.2	Skin corrosion/irritation	1B	Skin Corr. 1B	H314
3.3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis.

2.2 Label elements

Labelling

Signal word

Danger

Pictograms

GHS05, GHS07



Hazard statements

H302

Harmful if swallowed

H314

Causes severe skin burns and eye damage

Precautionary statements

Precautionary statements - prevention

P270

Do not eat, drink or smoke when using this product

P280

Wear protective gloves/eye protection

Precautionary statements - response

P303+P361+P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water

P305+P351+P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310

Immediately call a POISON CENTER/doctor

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

4-Nitrobenzyl chloride

Molecular formula

$C_7H_6ClNO_2$

Molar mass

171,6 g/mol

CAS No

100-14-1

EC No

202-822-7

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Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	1.809 mg/kg	oral

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

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

Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure.

Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

Following ingestion

Rinse mouth immediately and drink plenty of water. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects). Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Corrosion, Vomiting, Risk of blindness, Gastric perforation, Risk of serious damage to eyes

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

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

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

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Hazardous combustion products

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

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. 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.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal.

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

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

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

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

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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)

Country	Name of agent	CAS No	Identifier	TWA [mg/m ³]	STEL [mg/m ³]	Ceiling-C [mg/m ³]	Notation	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

Notation

Ceiling-C	Ceiling value is a limit value above which exposure should not occur
i	Inhalable fraction
r	Respirable fraction
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)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection. Wear face 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)

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- **material thickness**

>0,11 mm

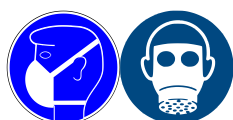
- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Form	powder, crystalline
Colour	whitish - light yellow
Odour	odourless
Melting point/freezing point	70 – 73 °C
Boiling point or initial boiling point and boiling range	not determined
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not applicable
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	not determined
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	this information is not available

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Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	not determined
Relative vapour density	Information on this property is not available.
Particle characteristics	No data available.
<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:	There is no additional information.

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

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

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 toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	1.809 mg/kg	rat		

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Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

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.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

• If in eyes

causes burns, Causes serious eye damage, risk of blindness

• If inhaled

Data are not available.

• If on skin

causes severe burns, causes poorly healing wounds

• Other information

none

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

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,212 mg/mg

Theoretical Oxygen Demand (with nitrification): 1,585 mg/mg

Theoretical Carbon Dioxide: 1,795 mg/mg

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

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.

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 4 irritant - skin irritation and eye damage

HP 6 acute toxicity

HP 8 corrosive

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.

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SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 3261
IMDG-Code	UN 3261
ICAO-TI	UN 3261

14.2 UN proper shipping name

ADRRID	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
IMDG-Code	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
ICAO-TI	Corrosive solid, acidic, organic, n.o.s.
Technical name	4-Nitrobenzyl chloride

14.3 Transport hazard class(es)

ADRRID	8
IMDG-Code	8
ICAO-TI	8

14.4 Packing group

ADRRID	II
IMDG-Code	II
ICAO-TI	II

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous 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.

14.8 Information for each of the UN Model Regulations

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

Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
Particulars in the transport document	UN3261, CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S., (4-Nitrobenzyl chloride), 8, II, (E)
Classification code	C4
Danger label(s)	8
	
Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 kg

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Transport category (TC)	2
Tunnel restriction code (TRC)	E
Hazard identification No	80
Emergency Action Code	2X

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

Classification code	C4
Danger label(s)	8



Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 kg
Transport category (TC)	2
Hazard identification No	80

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
Particulars in the shipper's declaration	UN3261, CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S., (4-Nitrobenzyl chloride), 8, II
Marine pollutant	-
Danger label(s)	8



Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 kg
EmS	F-A, S-B
Stowage category	B
Segregation group	1 - Acids

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

Proper shipping name	Corrosive solid, acidic, organic, n.o.s.
Particulars in the shipper's declaration	UN3261, Corrosive solid, acidic, organic, n.o.s., (4-Nitrobenzyl chloride), 8, II
Danger label(s)	8



Special provisions (SP)	A3
Excepted quantities (EQ)	E2

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Limited quantities (LQ)

5 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)

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
	not assigned		

Deco-Paint Directive

VOC content	0 %
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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
4-Nitrobenzyl chloride	Organohalogen compounds and substances which may form such compounds in 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

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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

not listed

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
CA	NDSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NDSL	Non-domestic Substances List (NDSL)
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
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
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Danger		yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.	yes
14.8		Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information	yes
14.8		Classification code: C4	yes
14.8		Danger label(s): 8	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Special provisions (SP): 274	yes
14.8		Excepted quantities (EQ): E2	yes
14.8		Limited quantities (LQ): 1 kg	yes
14.8		Transport category (TC): 2	yes
14.8		Hazard identification No: 80	yes
15.1	Restrictions according to REACH, Annex XVII		yes
15.1		Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table)	yes
15.1	List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed.		yes
15.1		National regulations(GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed	yes
15.1		Restrictions according to GB REACH, Annex 17: not listed	yes
15.1		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.	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
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)
Ceiling-C	Ceiling value
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 identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
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 (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	Short-term exposure limit
TWA	Time-weighted average
VOC	Volatile Organic Compounds

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Abbr.	Descriptions of used abbreviations
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
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.