

Safety data sheet

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



Isooctane ROTISOLV® ≥99,8 %, UV/IR-Grade

article number: **CP80**
Version: **4.0 en**
Replaces version of: 2021-08-16
Version: (3)

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

1.1 Product identifier

Identification of the substance	Isooctane ROTISOLV® ≥99,8 %, UV/IR-Grade
Article number	CP80
EC number	208-759-1
CAS number	540-84-1
Alternative name(s)	2,2,4-Trimethylpentane

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

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone:+49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: :Department Health, Safety and Environment

e-mail (competent person): **sicherheit@carlroth.de**

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	2	Flam. Liq. 2	H225
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.8D	Specific target organ toxicity - single exposure (narcotic effects, drowsiness)	3	STOT SE 3	H336
3.10	Aspiration hazard	1	Asp. Tox. 1	H304
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

The product is combustible and can be ignited by potential ignition sources. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling

Signal word

Danger

Pictograms

GHS02, GHS07,
GHS08, GHS09



Hazard statements

H225 Highly flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H336 May cause drowsiness or dizziness
H410 Very toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat, sparks, open flames, hot surfaces. No smoking
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection

Precautionary statements - response

P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting
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
P312 Call a POISON CENTRE/doctor if you feel unwell

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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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Isooctane
Molecular formula	C ₈ H ₁₈
Molar mass	114,2 g/mol
CAS No	540-84-1
EC No	208-759-1

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

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

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

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. Do not induce vomiting. Observe aspiration hazard if vomiting occurs. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Following inhalation: Drowsiness, Dizziness, Narcosis,
Following skin contact: Irritation,
After eye contact: Irritant effects,
Following ingestion: Aspiration hazard

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. 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. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: 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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

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

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.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

Measures to protect the environment

Avoid release to the environment.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ground/bond container and receiving equipment.

Ventilation requirements

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.

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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	2.035 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	773 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggles with side protection.

Skin protection



• hand protection

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

>0,3 mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

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• other protection measures

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

Flame-retardant protective clothing.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °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
Odour	like: Gasoline
Melting point/freezing point	-107 °C
Boiling point or initial boiling point and boiling range	99,2 °C at 1.013 hPa
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	45 g/m ³ (LEL) - 290 g/m ³ (UEL) / 1 vol% (LEL) - 6 vol% (UEL)
Flash point	-12 °C (ECHA)
Auto-ignition temperature	418 °C (ECHA) (auto-ignition temperature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	(neutral)
Kinematic viscosity	not determined
Dynamic viscosity	0,5 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	2,2 mg/l at 25 °C (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	4,08 (ECHA)
Soil organic carbon/water (log KOC)	2,38 (ECHA)
Vapour pressure	2,8 kPa at 20 °C

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Density and/or relative density

Density 0,69 g/cm³ at 15 °C

Relative vapour density 3,9 (air = 1)

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics:

Gas group (explosion group) IIA
Maximum Experimental Safe Gap value; MESG > 0,9 mm

Maximum explosion pressure 9 bar

Surface tension 18,77 mN/m (20 °C) (ECHA)

Refractive index 1,392

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.

If heated

Risk of ignition.

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

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. UV-radiation/sunlight.

10.5 Incompatible materials

different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	>5.000 mg/kg	rat		ECHA
inhalation: vapour	LC50	>33,52 mg/l/4h	rat		ECHA
dermal	LD50	>2.000 mg/kg	rabbit		ECHA

Skin corrosion/irritation

Causes skin irritation.

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

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

May be fatal if swallowed and enters airways.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, aspiration hazard

• If in eyes

causes slight to moderate irritation

• If inhaled

drowsiness, dizziness, fatigue, narcosis

• If on skin

causes skin irritation

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• Other information

none

11.2 Endocrine disrupting properties

Not listed.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LL50	18,4 mg/l	fish	ECHA	96 h
LC50	0,11 mg/l	fish	ECHA	96 h
EC50	0,4 mg/l	aquatic invertebrates	ECHA	48 h
EL50	2,4 mg/l	aquatic invertebrates	ECHA	48 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EL50	1,6 mg/l	aquatic invertebrates	ECHA	21 d
EC50	0,23 mg/l	aquatic invertebrates	ECHA	21 d

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand: 3,501 mg/mg

Theoretical Carbon Dioxide: 3,082 mg/mg

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	61,81 %	70 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

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n-octanol/water (log KOW)	4,08 (ECHA)
BCF	231 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2,38 (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

13.3 Remarks

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

SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 1262
IMDG-Code	UN 1262
ICAO-TI	UN 1262

14.2 UN proper shipping name

ADRRID	OCTANES
IMDG-Code	OCTANES





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ICAO-TI	Octanes
14.3 Transport hazard class(es)	
ADRRID	3
IMDG-Code	3
ICAO-TI	3
14.4 Packing group	
ADRRID	II
IMDG-Code	II
ICAO-TI	II
14.5 Environmental hazards	hazardous to the aquatic environment
14.6 Special precautions for user	
Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7 Maritime transport in bulk according to IMO instruments	
The cargo is not intended to be carried in bulk.	
14.8 Information for each of the UN Model Regulations	
Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information	
Proper shipping name	OCTANES
Particulars in the transport document	UN1262, OCTANES, 3, II, (D/E), environmentally hazardous
Classification code	F1
Danger label(s)	3, "Fish and tree"
	
Environmental hazards	yes (hazardous to the aquatic environment)
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	3YE
Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information	
Classification code	F1
Danger label(s)	3 Fish and tree
	



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Environmental hazards	Yes Hazardous to water
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	
Proper shipping name	OCTANES
Particulars in the shipper's declaration	UN1262, OCTANES, 3, II, -12°C c.c., MARINE POLLUTANT
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Danger label(s)	3, "Fish and tree"
	
Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-E, S-E
Stowage category	B
International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information	
Proper shipping name	Octanes
Particulars in the shipper's declaration	UN1262, Octanes, 3, II
Environmental hazards	YES (hazardous to the aquatic environment)
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)

Seveso Directive

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2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
E1	environmental hazards (hazardous to the aquatic environment, cat. 1)	100	200	56)

Notation

56) Hazardous to the Aquatic Environment in category Acute 1 or Chronic 1

Deco-Paint Directive

VOC content	100 % 690 g/l
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Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	690 g/l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

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

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

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
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

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

15.2 Chemical Safety Assessment

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

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SECTION 16: Other information

Indication of changes (revised safety data sheet)

Alignment to regulation:

Restructuring: section 9, section 14

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
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

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	Bioconcentration factor
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
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
EL50	Effective Loading 50 %: the EL50 corresponds to the loading rate required to produce a response in 50% of the test organisms
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

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Abbr.	Descriptions of used abbreviations
IMDG-Code	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
LL50	Lethal Loading 50 %: the LL50 corresponds to the loading rate causing 50 % lethality
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)
UEL	Upper explosion limit (UEL)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
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.