

Safety data sheet

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



3,3'-Diaminodiphenyl sulphone $\geq 99\%$ for synthesis

article number: **8082**
Version: **3.0 en**
Replaces version of: 19.10.2021
Version: (2)

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Revision: 02.03.2024

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

1.1 Product identifier

Identification of the substance	3,3'-Diaminodiphenyl sulphone $\geq 99\%$ for synthesis
Article number	8082
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
EC number	209-967-5
CAS number	599-61-1

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 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
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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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.8	Specific target organ toxicity - single exposure	2	STOT SE 2	H371
3.9	Specific target organ toxicity - repeated exposure	2	STOT RE 2	H373
4.1C	Hazardous to the aquatic environment - chronic hazard	2	Aquatic Chronic 2	H411

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Delayed or immediate effects can be expected after short or long-term exposure. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

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

Signal word

Warning

Pictograms

GHS07, GHS08,
GHS09



Hazard statements

H302	Harmful if swallowed
H371	May cause damage to organs (blood)
H373	May cause damage to organs (blood) through prolonged or repeated exposure
H411	Toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P260	Do not breathe dusts or mists
P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P273	Avoid release to the environment

Precautionary statements - response

P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell
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Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



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 $\geq 0,1\%$.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	3,3'-Diaminodiphenyl sulphone
Molecular formula	$C_{12}H_{12}N_2O_2S$
Molar mass	248,3 g/mol
CAS No	599-61-1
EC No	209-967-5

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

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	500 mg/kg	oral

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 all cases of doubt, or when symptoms persist, seek medical advice.

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 with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Vomiting

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, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

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

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 dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid dust formation.

Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

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.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

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.

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	2,5 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	2,5 mg/m ³	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	0,35 mg/m ³	human, inhalatory	worker (industry)	chronic - local effects
DNEL	0,35 mg/m ³	human, inhalatory	worker (industry)	acute - local effects
DNEL	0,35 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	0,01 mg/l	aquatic organisms	water	intermittent release
PNEC	0,004 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	10 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,041 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,004 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,006 mg/kg	terrestrial organisms	soil	short-term (single instance)

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

>0,11 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

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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
Colour	light brown
Odour	faintly perceptible
Melting point/freezing point	173 °C (ECHA)
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	>173 °C (ECHA)
pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	0,38 g/l at 36 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	0,76 (25 °C) (ECHA)
Soil organic carbon/water (log KOC)	1,76 (ECHA)
Vapour pressure	0,00002 hPa at 20 °C
<u>Density and/or relative density</u>	
Density	1,4 g/cm ³ at 20 °C (ECHA)

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Relative vapour density Information on this property is not available.

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

Surface tension 73,6 mN/m (20 °C) (ECHA)

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

Keep away from heat. Decomposition takes place from temperatures above: >173 °C.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
dermal	LD50	>2.000 mg/kg	rabbit		ECHA

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

May cause damage to organs (blood).

Hazard category	Target organ	Exposure route
2	blood	if exposed

Specific target organ toxicity - repeated exposure

May cause damage to organs (blood) through prolonged or repeated exposure.

Hazard category	Target organ	Exposure route
2	blood	if exposed

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

Data are not available.

• If in eyes

Data are not available.

• If inhaled

Data are not available.

• If on skin

Data are not available.

• Other information

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

11.2 Endocrine disrupting properties

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

11.3 Information on other hazards

There is no additional information.

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SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	$>100 \text{ mg/l}$	fish	ECHA	96 h
ErC50	$2,7 \text{ mg/l}$	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
LC50	$0,5 \text{ mg/l}$	aquatic invertebrates	ECHA	21 d
EC50	$>0,46 \text{ mg/l}$	aquatic invertebrates	ECHA	21 d

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): $1,804 \text{ mg/mg}$

Theoretical Oxygen Demand (with nitrification): $2,078 \text{ mg/mg}$

Theoretical Carbon Dioxide: $2,127 \text{ mg/mg}$

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	$>0 - <1 \%$	11 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	0,76 (25 °C) (ECHA)
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12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	1,76 (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

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

12.7 Other adverse effects

Data are not available.

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SECTION 13: Disposal considerations

13.1 Waste treatment methods



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

Sewage disposal-relevant information

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

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

Properties of waste which render it hazardous

HP 5 specific target organ toxicity (STOT)/aspiration toxicity
HP 6 acute toxicity
HP 14 ecotoxic

13.3 Remarks

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

SECTION 14: Transport information

14.1 UN number or ID number

ADR	UN 3077
IMDG-Code	UN 3077
ICAO-TI	UN 3077

14.2 UN proper shipping name

ADR	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
IMDG-Code	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
ICAO-TI	Environmentally hazardous substance, solid, n.o.s.
Technical name	3,3'-Diaminodiphenyl sulphone

14.3 Transport hazard class(es)

ADR	9
IMDG-Code	9
ICAO-TI	9

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14.4 Packing group

ADR	III
IMDG-Code	III
ICAO-TI	III

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

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

Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
Particulars in the transport document	UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (3,3'-Diaminodiphenyl sulphone), 9, III, (-)
Classification code	M7
Danger label(s)	9, "Fish and tree"
 	
Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	274, 335, 375, 601
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	3
Tunnel restriction code (TRC)	-
Hazard identification No	90

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
Particulars in the shipper's declaration	UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (3,3'-Diaminodiphenyl sulphone), 9, III
Marine pollutant	yes (hazardous to the aquatic environment), (3,3'-Diaminodiphenyl sulphone)
Danger label(s)	9, "Fish and tree"
 	
Special provisions (SP)	274, 335, 966, 967, 969

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Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
EmS	F-A, S-F
Stowage category	A

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

Proper shipping name	Environmentally hazardous substance, solid, n.o.s.
Particulars in the shipper's declaration	UN3077, Environmentally hazardous substance, solid, n.o.s., (3,3'-Diaminodiphenyl sulphone), 9, III
Environmental hazards	YES (hazardous to the aquatic environment)
Danger label(s)	9, "Fish and tree"
	
Special provisions (SP)	A97, A158, A179, A197, A215
Excepted quantities (EQ)	E1
Limited quantities (LQ)	30 kg

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

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
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200 500	57)

Notation

57) Hazardous to the Aquatic Environment in category Chronic 2

Deco-Paint Directive

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VOC content	0 %
VOC content	0 g/l

Industrial Emissions Directive (IED)

VOC content	0 %
VOC content	0 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

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	NDSL	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
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed

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Country	Inventory	Status
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
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
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)
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	VOC content: 0 % , 0 ^g /l	VOC content: 0 %	yes
15.1		VOC content: 0 ^g /l	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)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
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)

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Abbr.	Descriptions of used abbreviations
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	\equiv EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
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
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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.
Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). 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.
H371	May cause damage to organs (blood).
H373	May cause damage to organs (blood) through prolonged or repeated exposure.
H411	Toxic to aquatic life with long lasting effects.

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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.