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

3-Aminophenol ≥99%, for synthesis

article number: 0957 date of compilation: 2018-09-06 Version: 2.0 en Revision: 2022-07-01

Replaces version of: 2018-09-06

Version: (1)



Product identifier 1.1

Identification of the substance **3-Aminophenol** ≥99%, for synthesis

Article number 0957

EC number 209-711-2 CAS number 591-27-5

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

Relevant identified uses: Laboratory and analytical use

Laboratory chemical

Uses advised against: Do not use for products which come into contact

with foodstuffs. Do not use for private purposes

(household).

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 :Department Health, Safety and Environment

sheet:

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

Emergency telephone number 1.4

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
3.1I	Acute toxicity (inhal.)	4	Acute Tox. 4	H332
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

Spillage and fire water can cause pollution of watercourses.

2.2 **Label elements**

Labelling

Signal word Warning

Pictograms

GHS07, GHS09





Hazard statements

H302+H332 Harmful if swallowed or if inhaled

H411 Toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P260 Do not breathe dust/fume/gas/mist/vapours/spray

P273 Avoid release to the environment

P280 Wear protective gloves/protective clothing

Precautionary statements - response

P308+P313 IF exposed or concerned: Get medical advice/attention

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 3-Aminophenol

Molecular formula C₆H₇NO Molar mass 109,1 ^g/_{mol} CAS No 591-27-5 EC No 209-711-2

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

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	924 ^{mg} / _{kg} 1,5 ^{mg} / _l /4h	oral inhalation: dust/ mist

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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

Following inhalation: Cough, pain, choking, and breathing difficulties,

After eye contact: Irritant,

Following skin contact: Irritant effects, Following ingestion: Vomiting, Nausea

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, alcohol resistant 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 (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂)

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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.

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

Provision of sufficient ventilation. Avoid dust formation.

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

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted.

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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)

This information is not available.

Human health values

Relevant DNELs and other threshold levels					
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time	
DNEL	0,493 mg/m³	human, inhalatory	worker (industry)	chronic - systemic effects	
DNEL	2,5 mg/kg bw/ day	human, dermal	worker (industry)	chronic - systemic effects	

Environmental values

Relevant PNECs and other threshold levels

End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	1 ^{µg} / _I	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,1 ^{µg} / _l	aquatic organisms	marine water	short-term (single instance)
PNEC	96,19 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	12,6 ^{µg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	1,26 ^{µg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)
PNEC	1,93 ^{µg} / _{kg}	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

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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 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 scales

Colour white - whitish - grey

Odour odourless

Melting point/freezing point 116 – 122 °C (ECHA)

Boiling point or initial boiling point and boiling 284 °C at 990 hPa (ECHA)

range

Flammability this material is combustible, but will not ignite

readily

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Lower and upper explosion limit not determined Flash point 178 °C (ECHA) Auto-ignition temperature not determined

Decomposition temperature >300 °C

pH (value) 6,8 (in aqueous solution: $10^{9}/_{l}$, 20° C) (ECHA)

Kinematic viscosity not relevant

Solubility(ies)

Water solubility 20,1 ^g/_l at 20 °C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 0,183 (pH value: 7,5, 20 °C) (ECHA)

Vapour pressure ~0 Pa at 20 °C

Density and/or relative density

Density $1,276 \, {}^{9}/_{cm^3}$ at 20 °C (ECHA)

Relative vapour density information on this property is not available

Bulk density $\sim 700 \, \mathrm{kg/m^3}$

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical 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

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10.4 Conditions to avoid

Keep away from heat. Decompostion takes place from temperatures above: >300 °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 toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed. Harmful if inhaled.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	924 ^{mg} / _{kg}	rat		TOXNET
dermal	LD50	8.112 ^{mg} / _{kg}	rabbit		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

vomiting, nausea

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• If in eyes

slightly irritant but not relevant for classification

If inhaled

cough, pain, choking, and breathing difficulties

• If on skin

slightly irritant but not relevant for classification

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

Toxic to aquatic life with long lasting effects.

Endpoint	Value	Species	Source	Exposure time
LC50	>100 ^{mg} / _l	fish	ECHA	96 h
ErC50	67,7 ^{mg} / _l	algae	ECHA	72 h
EC50	41 ^{mg} / _l	algae	ECHA	72 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time	
LC50	>100 ^{mg} / _l	fish	ECHA	21 d	
EC50	0,116 ^{mg} / _l	aquatic invertebrates	ECHA	21 d	

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,419 $^{\rm mg}/_{\rm mg}$ Theoretical Oxygen Demand: 1,906 $^{\rm mg}/_{\rm mg}$ Theoretical Carbon Dioxide: 2,42 $^{\rm mg}/_{\rm mg}$

Process of degradabili	t١	ı
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Process	Degradation rate	Time
oxygen depletion	0 %	28 d

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12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	0,183 (pH value: 7,5, 20 °C) (ECHA)
BCF	4 (ECHA)

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

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 2512
IMDG-Code UN 2512
ICAO-TI UN 2512

14.2 UN proper shipping name

ADRRID AMINOPHENOLS
IMDG-Code AMINOPHENOLS

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	ICAO-TI	Aminophenols
14.3	Transport hazard class(es)	
	ADRRID	6.1
	IMDG-Code	6.1
	ICAO-TI	6.1
14.4	Packing group	
	ADRRID	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

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Proper shipping name	AMINOPHENOLS
Particulars in the transport document	UN2512, AMINOPHENOLS, 6.1, III, (E), environmentally hazardous
Classification code	T2
Danger label(s)	6.1, "Fish and tree"
Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	279, 802(ADN)

Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	2
Tunnel restriction code (TRC)	Е
Hazard identification No	60
Emergency Action Code	2X

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

Classification code	T2
Danger label(s)	6.1 Fish and tree

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Environmental hazards Ye

Hazardous to water

Special provisions (SP) 279, 802(ADN)

Excepted quantities (EQ) E1
Limited quantities (LQ) 5 kg
Transport category (TC) 2
Hazard identification No 60

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name AMINOPHENOLS

Particulars in the shipper's declaration UN2512, AMINOPHENOLS, 6.1, III, MARINE POL-

LUTANT

Marine pollutant yes (hazardous to the aquatic environment)

Danger label(s) 6.1, "Fish and tree"

Special provisions (SP) 279

Excepted quantities (EQ) E1

Limited quantities (LQ) 5 kg

EmS F-A, S-A

Stowage category A

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

Proper shipping name Aminophenols

Particulars in the shipper's declaration UN2512, Aminophenols, 6.1, III

Environmental hazards yes (hazardous to the aquatic environment)

Danger label(s) 6.1

Special provisions (SP) A113
Excepted quantities (EQ) E1
Limited quantities (LQ) 10 kg

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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/	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

VOC content 0 % 0 9/ _I

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

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

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	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AIIC

Australian Inventory of Industrial Chemicals List of Existing and New Chemical Substances (CSCL-ENCS)

CSCL-ENCS DSL ECSI IECSC INSQ KECI 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 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

Taiwan Chemical Substance Inventory

TCSI 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)

Alignment to regulation:

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.1		Classification acc. to GHS: change in the listing (table)	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.1		The most important adverse physicochemical, human health and environmental effects: Spillage and fire water can cause pollution of watercourses.	yes
2.2		Pictograms: change in the listing (table)	yes
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning		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	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In land Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concern ing the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
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 iden fier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	≡ 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
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 Na tions

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Abbr.	Descriptions of used abbreviations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
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
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

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

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

Code	Text
H302	Harmful if swallowed.
H332	Harmful if inhaled.
H411	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.

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