

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: **4530**
Version: **3.0 en**
Replaces version of: 2022-04-07
Version: (2)

date of compilation: 2017-02-15
Revision: 2024-03-02

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

1.1 Product identifier

Identification of the substance	3-Nitrobenzotrile $\geq 98\%$, for synthesis
Article number	4530
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	210-587-7
CAS number	619-24-9

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 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 Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	https://www.poisons.ie/

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: 4530

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

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.1O	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.1D	Acute toxicity (dermal)	4	Acute Tox. 4	H312
3.1I	Acute toxicity (inhal.)	4	Acute Tox. 4	H332
4.1C	Hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

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

Signal word

Warning

Pictograms

GHS07



Hazard statements

H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled
H412 Harmful to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P270 Do not eat, drink or smoke when using this product
P280 Wear protective gloves/protective clothing/eye protection/face protection

Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of 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

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



H412 Harmful to aquatic life with long lasting effects.

Safety data sheet

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



3-Nitrobenzonitrile $\geq 98\%$, for synthesis

article number: 4530

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	3-Nitrobenzonitrile
Molecular formula	$C_7H_4N_2O_2$
Molar mass	148,1 g/mol
CAS No	619-24-9
EC No	210-587-7

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	500 mg/kg >1.000 mg/kg 1,5 mg/l/4h	oral dermal inhalation: dust/ mist

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Rinse cautiously with water for several minutes.

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

Safety data sheet

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



3-Nitrobenzonitrile $\geq 98\%$, for synthesis

article number: 4530

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 (NO_x), 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 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.

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: 4530

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.

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. 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.

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



Safety data sheet

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



3-Nitrobenzonitrile $\geq 98\%$, for synthesis

article number: 4530

• 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

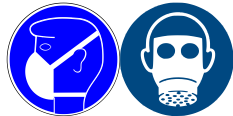
• breakthrough times of the glove material

>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	powder, crystalline
Colour	yellow
Odour	faintly perceptible
Melting point/freezing point	115 – 117 °C
Boiling point or initial boiling point and boiling range	164 – 166 °C
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

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: **4530**

pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	1,7 g/l at 25 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	1,17 (TOXNET) (Experimental data)
Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	0,33 g/cm ³ at 20 °C
Relative vapour density	Information on this property is not available.
Bulk density	~500 kg/m ³
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, Bases

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.

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: 4530

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. Harmful in contact with skin. Harmful if inhaled.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LDLo	50 mg/kg	rat		TOXNET
dermal	LD50	>1.000 mg/kg	guinea pig		TOXNET

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

Data are not available.

• If in eyes

Data are not available.

• If inhaled

Data are not available.

• If on skin

Frequently or prolonged contact with skin may cause dermal irritation

Safety data sheet

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



3-Nitrobenzonitrile $\geq 98\%$, for synthesis

article number: 4530

• Other information

Substance not yet fully tested.

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.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
EC50	48 mg/l	daphnia magna	ECOTOX	48 h
LC50	60 mg/l	Pimephales promelas	ECOTOX	96 h

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,188 mg/mg
Theoretical Oxygen Demand (with nitrification): 1,647 mg/mg
Theoretical Carbon Dioxide: 2,08 mg/mg

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,17 (TOXNET) (Experimental data)
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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.

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: 4530

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

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 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 | not subject to transport regulations |
| 14.2 | UN proper shipping name | not assigned |
| 14.3 | Transport hazard class(es) | none |
| 14.4 | Packing group | not assigned |
| 14.5 | Environmental hazards | non-environmentally hazardous acc. to the dangerous goods regulations |
| 14.6 | Special precautions for user | There is no additional information. |
| 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 | |
| | International Maritime Dangerous Goods Code (IMDG) - Additional information | Not subject to IMDG. |
| | International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information | Not subject to ICAO-IATA. |

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.

Safety data sheet

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



3-Nitrobenzonitrile ≥ 98 %, for synthesis

article number: 4530

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	100 %
VOC content	330 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.

Safety data sheet

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



3-Nitrobenzotrile ≥98 %, for synthesis

article number: 4530

National inventories

Country	Inventory	Status
CA	NDSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	ISHA-ENCS	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)

Legend

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)
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
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	VOC content: 100 % 330 g/l	VOC content: 100 %	yes
15.1		VOC content: 330 g/l	yes
15.1		National inventories: change in the listing (table)	yes

Safety data sheet

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



3-Nitrobenzotrile $\geq 98\%$, for synthesis

article number: 4530

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)
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)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
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
IMDG	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
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)
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). 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).

Safety data sheet

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



3-Nitrobenzonitrile $\geq 98\%$, for synthesis

article number: 4530

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

Code	Text
H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H332	Harmful if inhaled.
H412	Harmful 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.