

Chemical Safety Data Sheet MSDS / SDS

CACOTHELINE

Revision Date:2026-03-21 Revision Number:1

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

Product identifier

Product name : CACOTHELINE
CBnumber : CB0127493
CAS : 561-20-6
EINECS Number : 209-215-6
Synonyms : CACOTHELIN;nitrobrucine

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to....
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P271 Use only outdoors or in a well-ventilated area.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

No data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: CACOTHELINE
Synonyms	: CACOTHELIN;nitrobrucine
CAS	: 561-20-6
EC number	: 209-215-6
MF	: C21H21N3O7
MW	: 427.41

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately.

In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area.

Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-

approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

Body Protection

protective clothing

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	crystalline
b) Color	yellow
c) Odor	No data available
d) Melting point/freezing point	Melting point/range: > 300 °C
e) Initial boiling point and boiling range	542.58°C (rough estimate)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	1.4011 (rough estimate)
Relative density	1.4011 (rough estimate)
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 5,1 mg/kg (Expert judgment)

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Acute toxicity estimate Inhalation - 4 h - 0,1 mg/l - dust/mist(Expert judgment)

Acute toxicity estimate Inhalation - 4 h - 0,1 mg/l - dust/mist (Expert judgment)

Acute toxicity estimate Dermal - 5 mg/kg (Expert judgment)

Acute toxicity estimate Dermal - 5 mg/kg (Expert judgment)

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Causes damage to organs.

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2811

IMDG: 2811

IATA: 2811

14.2 UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (Cacotheline)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (Cacotheline)

IATA: Toxic solid, organic, n.o.s. (Cacotheline)

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

14.4 Packaging group

ADR/RID: I

IMDG: I

IATA: I

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (C/E)

Further information : No data available

SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No.

1907/2006.

National legislation

Seveso III: Directive 2012/18/EU of the H1 ACUTE TOXIC

European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

E1 ENVIRONMENTAL HAZARDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AIRC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

ATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC₅₀ - Half maximal inhibitory concentration

ICAO - International Civil Aviation Organization

IECSC - Inventory of Existing Chemical Substances in China

IMDG - International Maritime Dangerous Goods

IMO - International Maritime Organization

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardization

KECI - Korea Existing Chemicals Inventory

LC₅₀ - Lethal Concentration to 50 % of a test population

LD₅₀ - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pollution from Ships

n.o.s. - Not Otherwise Specified

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NZIoC - New Zealand Inventory of Chemicals

OECD - Organization for Economic Co-operation and Development

OPPTS - Office of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Substances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation

and Restriction of Chemicals

RID - Regulations concerning the International Carriage of Dangerous Goods by Rail

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - Taiwan Chemical Substance Inventory

TECI - Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (United States)

UN - United Nations

UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.