

Chemical Safety Data Sheet MSDS / SDS

N-Hexadecyltrimethylammonium chloride

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : N-Hexadecyltrimethylammonium chloride
CBnumber : CB2105341
CAS : 112-02-7
EINECS Number : 203-928-6
Synonyms : CETRIMONIUM CHLORIDE,CTAC

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 : 400-158-6606

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.

P391 Collect spillage. Hazardous to the aquatic environment

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

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.
P264 Wash hands thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H410 Very toxic to aquatic life with long lasting effects
H400 Very toxic to aquatic life
H335 May cause respiratory irritation
H319 Causes serious eye irritation
H318 Causes serious eye damage
H315 Causes skin irritation
H314 Causes severe skin burns and eye damage
H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: N-Hexadecyltrimethylammonium chloride
Synonyms	: CETRIMONIUM CHLORIDE,CTAC
CAS	: 112-02-7
EC number	: 203-928-6
MF	: C19H42ClN
MW	: 320

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NOx), Hydrogen chloride gas

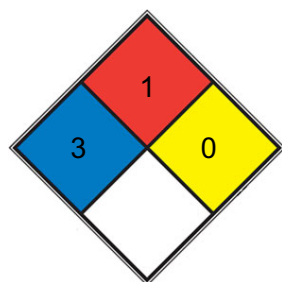
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place. hygroscopic

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

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

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	white powder
Odour	No data available
Odour Threshold	No data available
pH	pH(50g/l, 25°C) : 6.0~8.5
Melting point/freezing point	Melting point/range: 232 - 237 °C
Initial boiling point and boiling range	235 - 248 °C at 1.013 hPa - OECD Test Guideline 103
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	The product is not flammable. - A.10. (Regulation (EC) No 440/2008, Annex A)
Upper/lower flammability or explosive limits	No data available
Vapour pressure	< 0,01 hPa at 20 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	0,96 g/cm ³ at 20 °C -
Water solubility	0,24 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 3,08 at 25 °C - (calculated) - Bioaccumulation is not expected.
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Surface tension 33 mN/m at 1g/l - OECD Test Guideline 115

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen chloride gas

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 699 mg/kg (OECD Test Guideline 401)

Skin corrosion/irritation

Skin - Rabbit Result: Corrosive

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Causes serious eye damage. Eyes - Rabbit

Result: Corrosive

(OECD Test Guideline 405)

Respiratory or skin sensitisation

Buehler Test - Guinea pig Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

Escherichia coli/Salmonella typhimurium Result: negative

Mutagenicity (mammal cell test):

Chinese hamster fibroblasts Result: negative

Chromosome aberration test in vitro Chinese hamster fibroblasts

Result: negative

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rabbit - male and female - Dermal - 28 d - No observed adverse effect level - 10 mg/kg

Subacute toxicity

Repeated dose toxicity - Rat - male and female - Oral - 90 d - No observed adverse effect level - 113 mg/kg

Subchronic toxicity RTECS: ML9145000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Toxicity

LD50 skin in rabbit: 4300uL/kg/24H

SECTION 12: Ecological information

Toxicity

Toxicity to fish

static test LC50 - Danio rerio (zebra fish) - 0,19 - 0,29 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 0,280 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test NOEC - Pseudokirchneriella subcapitata (green algae) - 0,04 mg/l - 72 h
(OECD Test Guideline 201)

Remarks: (in analogy to similar products)

static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0,08 mg/l - 72 h
(OECD Test Guideline 201)

Remarks: (in analogy to similar products)

Toxicity to bacteria

static test EC50 - Pseudomonas putida - 0,96 mg/l - 16 h (DIN 38 412 Part 8)

Persistence and degradability

No data available

Bioaccumulative potential

Bioaccumulation *Lepomis macrochirus* (Bluegill sunfish) - 56 d (Cetrimonium chloride)

Bioconcentration factor (BCF): 79 Elimination: yes

(US-EPA)

Mobility in soil

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.

Other adverse effects

Very toxic to aquatic life with long lasting effects.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2923 IMDG: 2923 IATA: 2923

UN proper shipping name

ADR/RID: CORROSIVE SOLID, TOXIC, N.O.S. (Cetrimonium chloride)

IMDG: CORROSIVE SOLID, TOXIC, N.O.S. (Cetrimonium chloride) IATA: Corrosive solid, toxic, n.o.s. (Cetrimonium chloride)

Transport hazard class(es)

ADR/RID: 8 (6.1) IMDG: 8 (6.1) IATA: 8 (6.1)

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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