

Chemical Safety Data Sheet MSDS / SDS

(-)-COTININERevision Date:2023-05-20 Revision Number:1

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

Product name : (-)-COTININE
CBnumber : CB6402037
CAS : 486-56-6
EINECS Number : 207-634-9
Synonyms : Cotinine,(-)-Cotinine

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**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral
Skin irritation, Category 2
Eye irritation, Category 2
Specific target organ toxicity – single exposure, Category 3

Label elements**Pictogram(s)**

□□□□

Signal word : Danger

Hazard statement(s)

H225 Highly Flammable liquid and vapour
H302 Harmful if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation

H370 Causes damage to organs

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

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

P311 Call a POISON CENTER or doctor/physician.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

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

Continuerinsing.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P405 Store locked up.

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

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

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P319 Get medical help if you feel unwell.

Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: (-)-COTININE
Synonyms	: Cotinine,(-)-Cotinine
CAS	: 486-56-6
EC number	: 207-634-9
MF	: C10H12N2O
MW	: 176.22

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

SECTION 5: Firefighting measures

Extinguishing media

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

Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

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

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Solid
Colour	Colourless to Very Dark Orange Oil to
Odour	no data available
Melting point/freezing point	40-42°C
Boiling point or initial boiling point and boiling range	250°C(150 torr)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	>230 °F
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Sparingly), DMSO (Slightly), Methanol (Sparingly)
Partition coefficient n-octanol/water	log Kow = 0.07
Vapour pressure	0.000421mmHg at 25°C
Density and/or relative density	no data available
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Complete recovery of cotinine as $^{14}\text{CO}_2$ (N-methyl-labeled) was observed after 72 days incubation using sediment samples collected upstream and downstream from a municipal wastewater treatment plant outfall on Fourmile Creek near Ankeny, IA(1). However, caffeine exposure was shown to decrease cotinine biodegradation by 36 and 200% using sediments from Boulder Creek and the Platte River, respectively. Biodegradation proceeded via microbial demethylation of the N-methyl component of cotinine and is metabolic precursor, nicotine(1).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for cotinine(SRC), using a log Kow of 0.07(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of cotinine is estimated as 130(SRC), using a log Kow of 0.07(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that cotinine is expected to have high mobility in soil. Using a 2.4 m soil column packed with Mohall-Laveen sandy loam soil from an area northeast of Pheonix, AZ and a secondarily-treated effluent from a municipal waste treatment plant, cotinine concentrations were reported as 0.137 and below the reporting limit of 0.023 ug/L at the beginning and ending dates of May 29, 2001 and Jun 6, 2001, respectively. The concentration in the soil column drainage basin was 0.101 ug/L, collected on Jun 20, 2001(4).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1230 (For reference only, please check.)

IMDG: UN1230 (For reference only, please check.)

IATA: UN1230 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: METHANOL (For reference only, please check.)

IMDG: METHANOL (For reference only, please check.)

IATA: METHANOL (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

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

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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.