

Chemical Safety Data Sheet MSDS / SDS

TRANS-3'-HYDROXYCOTININE, METHYL-D3Revision Date:2026-03-21 Revision Number:1

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

Product name : TRANS-3'-HYDROXYCOTININE, METHYL-D3
CBnumber : CB1333660
CAS : 159956-78-2
Synonyms : rel-Hydroxycotinine-d3;trans-3'-Hydroxy Cotinine-d3

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

P311 Call a POISON CENTER or doctor/physician.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H370 Causes damage to organs
H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: TRANS-3'-HYDROXYCOTININE, METHYL-D3
Synonyms	: rel-Hydroxycotinine-d3;trans-3'-Hydroxy Cotinine-d3
CAS	: 159956-78-2
MF	: C10H9D3N2O2
MW	: 195.23

SECTION 4: 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

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

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

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

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

Specific hazards during fire fighting

Combustible. Pay attention to flashback. Vapors are heavier than air and may spread along floors. Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products

Nature of decomposition products not known.

Specific extinguishing methods

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

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

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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 with liquid-absorbent material. Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Avoidance of contact

Acid chlorides Acid anhydrides Oxidizing agents Alkali metals Reducing agents Acids

Storage

Further information on storage conditions

Keep container tightly closed in a dry and wellventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

3, Flammable liquids

Recommended storage temperature

-20 °C

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Further information: Skin

Biological occupational exposure limits

Engineering measures

No data available

Personal protective equipment**Respiratory protection**

required when vapours/aerosols 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 ABEK

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.

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 and body protection

Flame retardant antistatic protective clothing.

Hand protection**Remarks**

required

Hygiene measures

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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

White to Pale Yellow

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

No data available

Boiling point/boiling range

No data available

Flash point

9.7 °C (10 hPa)

Method: closed cup

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

No data available

Density

No data available

Water solubility

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

Not classified as explosive.

Oxidizing properties

none

Molecular weight

195.23 g/mol

Particle characteristics Particle size

No data available

Solubility

Chloroform (Slightly), Methanol (Slightly)

Physical state

Solid

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

Warming.

Incompatible materials

Acid chlorides Acid anhydrides Oxidizing agents Alkali metals Reducing agents Acids

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

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

Mixture causes damage to organs. - Eyes

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

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

11.2 Additional Information

Methyl alcohol may be fatal or cause blindness if swallowed., Effects due to ingestion may include:, Headache, Dizziness, Drowsiness,
Chemical Book

metabolic acidosis, Coma,

Seizures., Symptoms may be delayed., Damage of the:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

Ecotoxicity

Components:

Methanol:

Toxicity to fish

LC50 (Lepomis macrochirus (Bluegill)): 15,400.0 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: US-EPA

Toxicity to daphnia and other aquatic invertebrates

EC50 (Daphnia magna (Water flea)): 18,260 mg/l End point: Immobilization Exposure time: 96 h Test Type: semi-static test Method: OECD Test Guideline 202

Toxicity to algae/aquatic plants

ErC50 (Pseudokirchneriella subcapitata (green algae)): ca. 22,000.0 mg/l Exposure time: 96 h Test Type: static test Method: OECD Test Guideline 201

Toxicity to fish (Chronic toxicity)

NOEC (Oryzias latipes (Orange-red killifish)): 7,900 mg/l Exposure time: 200 h Remarks: (External MSDS)

Toxicity to microorganisms

IC50 (activated sludge): > 1,000 mg/l Exposure time: 3 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 209

Persistence and degradability

Components:

Methanol:

Biodegradability

Result: Readily biodegradable. Biodegradation: 99 % Exposure time: 30 d Method: OECD Test Guideline 301D

Biochemical Oxygen Demand (BOD)

600 - 1,120 mg/g Incubation time: 5 d Remarks: (IUCLID)

Chemical Oxygen Demand (COD)

1,420 mg/g Remarks: (IUCLID)

ThOD

1,500 mg/g Remarks: (Lit.)

BOD/ThOD

76 % Remarks: Closed Bottle test (IUCLID)

Stability in water

Hydrolysis: 83 - 91 % at 19 °C(72 h) Remarks: Hydrolyzes on contact with water. Hydrolyzes readily. Degradation half life: 2.2 yr Remarks:

reaction with hydroxyl radicals (IUCLID)

Photodegradation

Degradation (direct photolysis): 50 % Degradation half life: 17.2 d

Bioaccumulative potential

Components:

Methanol:

Bioaccumulation

Species: Cyprinus carpio (Carp) Bioconcentration factor (BCF): 1.0 Exposure time: 72 d Temperature: 20 °C Concentration: 5 mg/l

Partition coefficient: noctanol/water

log Pow: -0.77 (25 °C) Method: (experimental) Remarks: (HSDB) Bioaccumulation is not expected.

Mobility in soil

Components:

Methanol:

Stability in soil

Remarks: Will not adsorb on soil.

Other adverse effects

Components:

Methanol:

Results of PBT and vPvB assessment

Substance is not persistent, bioaccumulative, and toxic (PBT).

Additional ecological information

Avoid release to the environment.

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 1230

Proper shipping name : Methanol

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : Class 3 - Flammable liquids, Division 6.1 - Toxic substances

Packing instruction (cargo aircraft) : 364

Packing instruction (passenger aircraft) : 352

IMDG-Code

UN number : UN 1230

Proper shipping name : METHANOL

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : 3 (6.1)

EmS Code : F-E, S-D

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : UN 1230

Proper shipping name : METHANOL

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : 3 (6.1)

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

No. / Code Chemical name / Category Threshold quantity

W5.3 Flammable liquids 1,000 t

Hazardous Chemicals for Priority Management

Not applicable under SAWS

Catalogue of Specially Controlled Hazardous

Listed Chemicals

List of Explosive Precursors

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not applicable

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222212769

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

Regulations on the Administration of Controlled Chemicals

List of Controlled Chemicals

Not listed

Regulations of Ozone Depleting Substances Management

List of Controlled Ozone Depleting Substances

Not listed

List of Controlled Ozone Depleting Substances Import and Export

Not listed

Environmental Protection Law

List of Priority Controlled Chemicals

Not listed

List of Key Controlled New Pollutants

Not listed

SECTION 16: Other information

Full text of other abbreviations

ACGIH

USA. ACGIH Threshold Limit Values (TLV)

ACGIH BEI

ACGIH - Biological Exposure Indices (BEI)

GBZ 2.1-2007

Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.

ACGIH / TWA

8-hour, time-weighted average

ACGIH / STEL

Short-term exposure limit

GBZ 2.1-2007 / PC-TWA

Permissible concentration - time weighted average

GBZ 2.1-2007 / PC-STEL AIC - Australian Invent Transport by Land of Bra bw - Body weight; **CMR** Standard of the German List (Canada); **ECx** - Conc associated with x% respo Chemical Substances (Jap response; **ERG** - Emerge GLP - Good Laboratory P cer; **IATA** - International Construction and Equipm Half maximal inhibitory c tion; **IECSC** - Inventory o tional Maritime Dangerou Industrial Safety and H Standardization; **KECI** - K tration to 50 % of a test (Median Lethal Dose); **MA** lution from Ships; **n.o.s.** No Observed (Adverse) E fect Level; **NOELR** - No Norm; **NTP** - National Toxi icals; **OECD** - Organizatio fice of Chemical Safety a and Toxic substance; **PIC** stances; **(Q)SAR** - (Quant (EC) No 1907/2006 of th Registration, Evaluation, Accelerating Decompositi Chemical Substance Inve Thailand Existing Chemicala States); **UN** - United Nat Transport of Dangerous **WHMIS** - Workplace Hazar Permissible concentration - short term exposure limit ry of Industrial Chemicals

ANTT - National Agency for il

ASTM - American Society for the Testing of Materials

- Carcinogen, Mutagen or Reproductive Toxicant

DIN nstitute for Standardisation

DSL - Domestic Substances ntration associated with x% response

ELx - Loading rate se

EmS - Emergency Schedule

ENCS - Existing and New n)

ErCx - Concentration associated with x% growth rate cy Response Guide

GHS - Globally Harmonized System

actice

IARC - International Agency for Research on Canir Transport Association

IBC - International Code for the nt of Ships carrying Dangerous Chemicals in Bulk

IC50 ncentration

ICAO - International Civil Aviation Organiza- Existing Chemical Substances in China

IMDG - International Maritime Organization
 IMO - International Maritime Organization
 ISHL - International Safety Law (Japan)
 ISO - International Organisation for Standardisation
 LC50 - Lethal Concentration
 LD50 - Lethal Dose to 50% of a test population
 POL - International Convention for the Prevention of Pollution
 Not Otherwise Specified
 NCh - Chilean Norm
 NO(A)EC - No Observed Effect Concentration
 NO(A)EL - No Observed (Adverse) Effect Level
 NOM - Official Mexican Standard
 NZIC - New Zealand Inventory of Chemicals
 OPPTS - Office of Pollution Prevention and Control
 PBT - Persistent, Bioaccumulative and Toxic
 Philippines Inventory of Chemicals and Chemical Substances
 Structure Activity Relationship
 REACH - Regulation of the European Parliament and of the Council concerning the restriction and restriction of Chemicals
 SADT - Self-heating Temperature
 SDS - Safety Data Sheet
 TCSI - Taiwanese Chemical Safety Information
 TDG - Transportation of Dangerous Goods
 TSCA - Toxic Substances Control Act (United States)
 UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods
 vPvB - Very Persistent and Very Bioaccumulative
 GHS - Globally Harmonized System of Classification and Labelling of Chemicals

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.