

Chemical Safety Data Sheet MSDS / SDS

GRAYANOTOXIN III

Revision Date:2026-03-20 Revision Number:1

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

Product identifier

Product name : GRAYANOTOXIN III
CBnumber : CB7674097
CAS : 4678-45-9
Synonyms : andromedol ;deacylasebotoxini

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

P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P405 Store locked up.
P501 Dispose of contents/container to.....
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P312 Call a POISON CENTER or doctor/physician if you feel unwell.
P322 Specific measures (see ...on this label).
P361 Remove/Take off immediately all contaminated clothing.
P363 Wash contaminated clothing before reuse.
P405 Store locked up.
P501 Dispose of contents/container to.....
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P321 Specific treatment (see ... on this label).
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.
P362 Take off contaminated clothing and wash before reuse.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.
P311 Call a POISON CENTER or doctor/physician.
P321 Specific treatment (see ... on this label).
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/container to.....

Hazard statements

H301 Toxic if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation
H331 Toxic if inhaled
H311 Toxic in contact with skin

SECTION 3: Composition/information on ingredients

Substance

Product name : GRAYANOTOXIN III
Synonyms : andromedol ;deacylasebotoxini
CAS : 4678-45-9
MF : C20H34O6
MW : 370.48

SECTION 4: First aid measures

Description of first aid measures

General information

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

After inhalation

Supply fresh air; consult doctor in case of complaints.

After skin contact

Immediately rinse with water.

After eye contact

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

After swallowing

Immediately call a doctor.

Most important symptoms and effects, both acute and delayed

No further relevant information available.

Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing agents

CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

No further relevant information available.

Advice for firefighters

Protective equipment

No special measures required.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Environmental precautions

Dilute with plenty of water.

Do not allow to enter sewers/ surface or ground water.

Methods and material for containment and cleaning up

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Dispose contaminated material as waste according to section 13.

Ensure adequate ventilation.

Protective Action Criteria for Chemicals

PAC-1

75-05-8 Acetonitrile 13 ppm

PAC-2

75-05-8 Acetonitrile 50 ppm

PAC-3

75-05-8 Acetonitrile 150 ppm

Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

Precautions for safe handling

No special precautions are necessary if used correctly.

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

Avoid prolonged or repeated exposure.

Keep away from sources of ignition.

Take precautionary measures against static discharge.

Information about protection against explosions and fires

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

Conditions for safe storage, including any incompatibilities

Storage

Store in accordance with information listed on the product insert.

Requirements to be met by storerooms and receptacles

Store in a cool location.

Information about storage in one common storage facility

Not required.

Further information about storage conditions

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

Specific end use(s)

No further relevant information available.

SECTION 8: Exposure controls/personal protection

Control parameters

Components with limit values that require monitoring at the workplace:

The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.

At this time, the remaining constituent has no known exposure limits.

75-05-8 Acetonitrile	
PEL	Long-term value: 70 mg/m ³ , 40 ppm
REL	Long-term value: 34 mg/m ³ , 20 ppm
TLV	Long-term value: 20 ppm Skin, A4

Additional information

The lists that were valid during the creation were used as basis.

Exposure controls

Appropriate engineering controls

No further data; see section 7.

Personal protective equipment

General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes.

Avoid contact with the eyes and skin.

Breathing equipment

Not required.

Protection of hands

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection

Tightly sealed goggles

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State

Liquid

Color

According to product specification

Odor

Characteristic

Structural Formula

C₂₀H₃₄O₆

Molecular Weight

370.5 g/mol

Storage Buffer

Odor Threshold

Not determined.

Formulation

A solution in water:acetonitrile

Melting point/Melting range

Undetermined.

Boiling point/Boiling range

81 °C (177.8 °F)

Flammability

Highly flammable.

Explosion limits

Lower: 4.4 Vol %

Upper: 16 Vol %

Flash point

2 °C (35.6 °F)

Auto igniting

525 °C (977 °F)

Decomposition temperature

Not determined.

pH

Not determined.

Viscosity

Kinematic

Not determined.

SOLUBILITY

Acetonitrile: Slightly Soluble: 0.1-1 mg/ml

Water: Slightly Soluble: 0.1-1 mg/ml

Dynamic

Not determined.

Solubility in / Miscibility with

Acetonitrile: Slightly Soluble: 0.1-1 mg/ml

Water: Slightly Soluble: 0.1-1 mg/ml

Water

Fully miscible.

Partition coefficient (n-octanol/water)

Not determined.

Vapor Pressure at 20 °C (68 °F)

98.6 hPa (74 mm Hg)

Vapor Pressure at 50 °C (122 °F)

330 hPa (247.5 mm Hg)

Density

1.36±0.1 g/cm³(Predicted)

Relative Density

1.36±0.1 g/cm³(Predicted)

Vapor Density

Not determined.

Particle characteristics

Not applicable.

Other information

Appearance

Form

Liquid

Important information on protection of health and environment, and on safety.

Ignition temperature

Product is not selfigniting.

Danger of explosion

Product is not explosive. However, formation of explosive air/vapor mixtures are possible.

VOC content

0.00 % 0.0 g/l / 0.00 lb/gal

Solids content

0.1 %

Change in condition

Evaporation Rate

Not determined.

SECTION 10: Stability and reactivity

Reactivity

No further relevant information available.

Chemical stability

Thermal decomposition / conditions to be avoided

No decomposition if used according to specifications.

Possibility of hazardous reactions

No dangerous reactions known.

Conditions to avoid

No further relevant information available.

Incompatible materials

No further relevant information available.

Hazardous decomposition products

No dangerous decomposition products known.

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD/LC50 values that are relevant for classification:

Substance / Estimate	Route	Endpoint	Value
ATE (Acute Toxicity Estimate)	Oral	LD50	1,220 mg/kg (mouse)
ATE (Acute Toxicity Estimate)	Dermal	LD50	2,973 mg/kg (rabbit)
ATE (Acute Toxicity Estimate)	Inhalative	LC50/4 h	21.1 mg/l
75-05-8 Acetonitrile	Oral	LD50	617 mg/kg (mouse) (OECD Test Guideline 401)
75-05-8 Acetonitrile	Dermal	LD50	1,500 mg/kg (rabbit) (Expert Judgement) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
75-05-8 Acetonitrile	Inhalative	LC50/4 h	6.022 mg/l (mouse) (OECD Test Guideline 403)
4678-45-9 Grayanotoxin III	Intraperitoneal	TDLO	0.015 mg/kg (rat)
4678-45-9 Grayanotoxin III	Intraperitoneal	LD50	840 mg/kg (mouse)

Primary irritant effect

on the skin

No irritant effect.

on the eye

Irritating effect.

Sensitization

No sensitizing effects known.

Additional toxicological information

The product shows the following dangers according to internally approved calculation methods for preparations

Harmful

Irritant

Interactive effects

No interactive effects between components are known.

Carcinogenic categories

IARC (International Agency for Research on Cancer)

None of the ingredients is listed.

NTP (National Toxicology Program)

None of the ingredients is listed.

OSHA-Ca (Occupational Safety & Health Administration)

None of the ingredients is listed.

Alternative sources for toxicological information

No non-standard sources for toxicological information where used.

SECTION 12: Ecological information

Toxicity

Aquatic toxicity

No further relevant information available.

Persistence and degradability

No further relevant information available.

Bioaccumulative potential

No further relevant information available.

Mobility in soil

No further relevant information available.

Results of PBT and vPvB assessment

PBT

Not applicable.

vPvB

Not applicable.

PBT:

Not applicable.

vPvB:

Not applicable.

Other adverse effects

Additional ecological information

General notes

Water hazard class 2 (Self-assessment) hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

SECTION 13: Disposal considerations

Waste treatment methods

Recommendation

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

Uncleaned packagings

Recommendation

Disposal must be made according to official regulations.

Recommended cleansing agent

Water, if necessary with cleansing agents.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA UN1993

UN proper shipping name

DOT Flammable liquids, n.o.s. (Acetonitrile)

IMDG FLAMMABLE LIQUID, N.O.S. (ACETONITRILE)

IATA Flammable liquid, n.o.s. (ACETONITRILE)

Transport hazard class(es)

DOT

Class: 3 Flammable liquids

Label: 3

IMDG, IATA

Class: 3 Flammable liquids

Label: 3

Packing group

DOT, IMDG, IATA II

Environmental hazards

Not applicable.

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable.

Transport/Additional information**DOT:****Quantity limitations**

On passenger aircraft/rail: 5 L

On cargo aircraft only: 60 L

IMDG:**Limited quantities (LQ)**

1L

Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

IATA:**Remarks**

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of

E1, E2, E4, or E5, this item meets the De Minimis

Quantities exemption, per IATA 2.6.10.

Therefore packaging does not have to be labeled as

Dangerous Goods/Excepted Quantity.

Special precautions for user

Warning: Flammable liquids

Hazard identification number (Kemler code)

EMS Number

F-E, S-E

Stowage Category

B

UN "Model Regulation"

UN 1993 FLAMMABLE LIQUID, N.O.S.

(ACETONITRILE), 3, II

SECTION 15: Regulatory information**Safety, health and environmental regulations/legislation specific for the substance or mixture**

No further relevant information available.

Sara

Section 355 (extremely hazardous substances):	None of the ingredients is listed.
Section 313 (Specific toxic chemical listings):	75-05-8 Acetonitrile
TSCA (Toxic Substances Control Act):	75-05-8 Acetonitrile ACTIVE
7732-18-5 Water ACTIVE	
Hazardous Air Pollutants 75-05-8 Acetonitrile	
Chemicals known to cause cancer:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for females:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for males:	None of the ingredients is listed.
Chemicals known to cause developmental toxicity:	None of the ingredients is listed.

Carcinogenic categories

EPA (Environmental Protection Agency):

75-05-8

Acetonitrile CBD, D

TLV (Threshold Limit Value)**75-05-8**

Acetonitrile A4

NIOSH-Ca (National Institute for Occupational Safety and Health)

None of the ingredients is listed.

Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Flammable liquids 2: Flammable liquids – Category 2

Acute toxicity - oral 4: Acute toxicity – Category 4

Eye irritation 2A: Serious eye damage/eye irritation – Category 2A

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.