

Chemical Safety Data Sheet MSDS / SDS

ADENOSINE 5'-O-(2-THIODIPHOSPHATE) TRILITHIUM SALTRevision Date:2026-05-31 Revision Number:1

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

Product name : ADENOSINE 5'-O-(2-THIODIPHOSPHATE) TRILITHIUM SALT
CBnumber : CB6333175
CAS : 73536-95-5
EINECS Number : 277-530-6
Synonyms : ADP-BETA-S;Ado-5'-PP[S]

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

Warning

Precautionary statements

No data available

Hazard statements

H371 May cause damage to organs

H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients**Substance**

Product name : ADENOSINE 5'-O-(2-THIODIPHOSPHATE) TRILITHIUM SALT

Synonyms	: ADP-BETA-S;Ado-5'-PP[S]
CAS	: 73536-95-5
EC number	: 277-530-6
MF	: C10H16LiN5O9P2S
MW	: 451.21

SECTION 4: First aid measures

General advice

Show this safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

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

In case of eye contact

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

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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) 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

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

Hazardous combustion products

Carbon oxides Nitrogen oxides (NOx) Sulphur oxides Oxides of phosphorus Lithium oxides

Specific extinguishing methods

Suppress (knock down) gases/vapours/mists with a water spray jet. 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: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. 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.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7: Handling and storage

Handling

Avoidance of contact

Strong oxidizing agents

Storage

Further information on storage conditions

Tightly closed. Dry. Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class

11, Combustible Solids

Recommended storage temperature

-20 °C

Further information on storage stability

Keep in a dry place.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Biological occupational exposure limits sure ceases)

Engineering measures

No data available

Personal protective equipment

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 P2

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

protective clothing

Hand protection

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Full contact

Manufacturer

KCL 741 L

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Splash contact

Manufacturer

KCL 741 L

Remarks

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).

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

powder

Color

white

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

No data available

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

water: 20mg/mL

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

No data available

Oxidizing properties

No data available

Molecular weight

461.07 g/mol

Particle characteristics Particle size

No data available

Solubility

water: 20 mg/mL

Physical state

White solid

SECTION 10: Stability and reactivity

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.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

no information available

Incompatible materials

Strong oxidizing agents

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 - 1,669 mg/kg (Calculation method)

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - > 40 mg/l - vapour(Calculation method)

Acute toxicity estimate Dermal - > 5,000 mg/kg (Calculation method)

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

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

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

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

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

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

acetone:**Toxicity to fish**

LC50 (*Pimephales promelas* (fathead minnow)): 6,210 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

LC50 (*Daphnia pulex* (Water flea)): 8,800 mg/l End point: mortality Exposure time: 48 h Test Type: static test Remarks: (ECHA)

Toxicity to algae/aquatic plants

NOEC (*M.aeruginosa*): 530 mg/l Exposure time: 8 d Test Type: static test Method: DIN 38412 Remarks: (maximum permissible toxic

concentration) (IUCLID)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

NOEC (Daphnia magna (Water flea)): 2,212 mg/l End point: reproduction rate Exposure time: 28 d Test Type: flow-through test Remarks: (ECHA)

Toxicity to microorganisms

EC50 (activated sludge): 61.15 mg/l Exposure time: 30 min Test Type: static test Method: OECD Test Guideline 209

ethanol:

Toxicity to fish

LC50 (Pimephales promelas (fathead minnow)): 15,300 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

LC50 (Ceriodaphnia dubia (water flea)): 5,012 mg/l End point: mortality Exposure time: 48 h Test Type: static test Remarks: (ECHA)

Toxicity to algae/aquatic plants

ErC50 (Chlorella vulgaris (Fresh water algae)): 275 mg/l Exposure time: 72 h Test Type: static test Method: OECD Test Guideline 201

Toxicity to fish (Chronic toxicity)

NOEC (Danio rerio (zebra fish)): 250 mg/l Exposure time: 120 h Test Type: semi-static test Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

NOEC (Daphnia magna (Water flea)): 9.6 mg/l End point: reproduction rate Exposure time: 9 d Test Type: semi-static test Remarks: (ECHA)

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

The value is given in analogy to the following substances: Methanol

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: Hydrolyses on contact with water. Hydrolyses readily. Degradation half life: 2.2 yr Remarks: reaction with hydroxyl radicals (IUCLID)

Photodegradation

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

acetone:

Biodegradability

aerobic Inoculum: activated sludge Result: Readily biodegradable. Biodegradation: 91 % Exposure time: 28 d Method: OECD Test Guideline 301B

Biochemical Oxygen Demand (BOD)

1,850 mg/g Incubation time: 5 d Remarks: (IUCLID)

Chemical Oxygen Demand (COD)

2,070 mg/g Remarks: (IUCLID)

ThOD

2,200 mg/g Remarks: (Lit.)

ethanol:

Biodegradability

aerobic Inoculum: activated sludge, non-adapted Result: Readily biodegradable. Biodegradation: ca. 95 % Exposure time: 15 d Method: OECD Test Guideline 301E

Biochemical Oxygen Demand (BOD)

930 - 1,670 mg/g Incubation time: 5 d Remarks: (Lit.)

ThOD

2,100 mg/g Remarks: (Lit.)

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.

acetone:

Bioaccumulation

Bioconcentration factor (BCF): < 10 Remarks: Does not bioaccumulate.

ethanol:

Bioaccumulation

Remarks: Due to the distribution coefficient noctanol/water, accumulation in organisms is not expected.

Partition coefficient: noctanol/water

log Pow: -0.35 (24 °C) pH: 7.4 Method: OECD Test Guideline 107 Remarks: 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

Not persistent, bioaccumulative, and toxic (PBT).

Additional ecological information

Avoid release to the environment.

acetone:

Results of PBT and vPvB assessment

Not persistent, bioaccumulative, and toxic (PBT). Not very persistent and very bioaccumulative (vPvB). : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

ethanol:

Results of PBT and vPvB assessment

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

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

Not regulated as a dangerous good

UN/ID No. : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Packing instruction (cargo aircraft) : Not applicable

Packing instruction (passenger aircraft) : Not applicable

IMDG-Code

Not regulated as a dangerous good

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

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 Regulations

JT/T 617

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Environmentally hazardous : no

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport 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

Hazardous Chemicals for Priority Management

Listed 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

B1A222215918 B1A222225598

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)

CN BEI

China. Biological Occupational Exposure Indices

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 AIIIC - 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 Standardisation; KECl - K tration to 50 % of a test (Median Lethal Dose); MA lution from Ships; MERC of Dangerous Goods; n.o. - No Observed (Adverse) fect Level; NOELR - No Norm; NTP - National Toxi icals; OECD - Organisatio 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 Chemica 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 Harmonised 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 - Interna- Goods

IMO - International Maritime Organisation

ISHL alth Law (Japan)

ISO - International Organisation for rea Existing Chemicals Inventory

LC50 - Lethal Concenopulation

LD50 - Lethal Dose to 50% of a test population POL - International Convention for the Prevention of Pol- SUR - The Agreement for the Facilitation of the Transport . - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Loading Rate

NOM - Official Mexican Order Program

NZIC - New Zealand Inventory of Chemicals for Economic Co-operation and Development

OPPTS - Office of Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic - Philippines Inventory of Chemicals and Chemical Substances Structure Activity Relationship

REACH - Regulation European Parliament and of the Council concerning the authorization and Restriction of Chemicals

SADT - Self-Heating Temperature

SDS - Safety Data Sheet

TCSI - Taiwanese Chemical Inventory

TDG - Transportation of Dangerous Goods

TECIS Inventory

TSCA - Toxic Substances Control Act (United States)

UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

Global Harmonized System of Classification and Labeling 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.