Chemical Safety Data Sheet MSDS / SDS

2-Cyanoethyl N,N,N',N'-tetraisopropylphosphorodiamidite

Revision Date: 2025-02-01 Revision Number: 1

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

Product identifier

Product name : 2-Cyanoethyl N,N,N',N'-tetraisopropylphosphorodiamidite

CBnumber : CB1231672

CAS : 102691-36-1

EINECS Number : 600-337-9

Synonyms : P-Reagent,2-cyanoethyl tetraisopropylphosphorodiamidite

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

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

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

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

P264 Wash hands thoroughly after handling.

P264 Wash skin thouroughly after handling.

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

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

P284 Wear respiratory protection.

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.

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

P370+P378 In case of fire: Use ... for extinction.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container to.....

Hazard statements

H226 Flammable liquid and vapour

H302 Harmful if swallowed

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H319 Causes serious eye irritation

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name : 2-Cyanoethyl N,N,N',N'-tetraisopropylphosphorodiamidite

Synonyms : P-Reagent,2-cyanoethyl tetraisopropylphosphorodiamidite

CAS : 102691-36-1
EC number : 600-337-9
MF : C15H32N3OP

MW : 301.41

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

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

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

Notes to physician

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

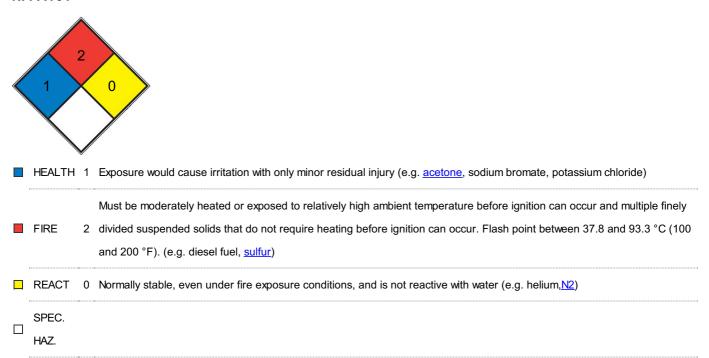
Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NOx), Oxides of phosphorus Combustible.

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary. Use water spray to cool unopened containers.

NFPA 704



SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

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

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

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 inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature -20 °C Handle and store under inert gas.

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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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	light yellow viscous
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	Melting point/freezing point: ca.12.7 °C at ca.1,013 hPa - OECD Test Guideline 102
Initial boiling point and boiling range	105 - 107 °C at 5.3 hPa - OECD Test Guideline 103
Flash point	48.5 °C - closed cup - ISO 3679
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	< 0.1 hPa at 25 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	0.949 g/cm3 at 25 °C - lit.
Water solubility	Hydrolysis
Partition coefficient: n-octanol/water	log Pow: 3.444 at 25 °C Bioaccumulation is not expected.
Autoignition temperature	No data available
Decomposition temperature	150 °C - Heating may cause an explosion.
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong bases, Strong oxidizing agents, Humid air, Water, air

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Oxides of phosphorus 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 - female - 500 mg/kg

(OECD Test Guideline 423)

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE)

Result: No skin irritation - 1 h (OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - In vitro study

Result: No eye irritation - 6 h (OECD Test Guideline 492)

Respiratory or skin sensitisation

(OECD Test Guideline 429)

Germ cell mutagenicity

Ames test

S. typhimurium 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

RTECS: Not available

Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting.

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

SECTION 12: Ecological information

Toxicity

No data available

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 - Daphnia magna Straus - 22.8 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test ErC50 - Pseudokirchneriella subcapitata - 20.4 mg/l - 72 h (OECD Test Guideline 201)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 0 % - Not readily biodegradable. (OECD Test Guideline 301F)

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

Harmful to aquatic life with long lasting effects. No data available

Stability in water DT50 - 28.6 min at 22 °C at 22 °C

(OECD Test Guideline 111)

Remarks: Hydrolyses on contact with water.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 1993 IMDG: 1993 IATA-DGR: 1993

UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (2-Cyanoethyl N,N,N',N'-

tetraisopropylphosphorodiamidite)

IMDG: FLAMMABLE LIQUID, N.O.S. (2-Cyanoethyl N,N,N',N'-

tetraisopropylphosphorodiamidite)

IATA-DGR: Flammable liquid, n.o.s. (2-Cyanoethyl N,N,N',N'- tetraisopropylphosphorodiamidite)

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA-DGR: 3

Packaging group

ADR/RID: III IMDG: III IATA-DGR: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA-DGR: no

Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport. Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

Incompatible materials

Strong bases, Strong oxidizing agents, Humid air, Water, air

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

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

EC Inventory: Not Listed.

Vietnam National Chemical Inventory: Not Listed. website: https://chemicaldata.gov.vn/

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

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: https://echa.europa.eu/

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/

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] ChemlDplus, 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:

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.