

## 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**

P501 Dispose of contents/container to....  
P403+P235 Store in a well-ventilated place. Keep cool.  
P370+P378 In case of fire: Use ... for extinction.  
P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
P284 Wear respiratory protection.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P240 Ground/bond container and receiving equipment.  
P233 Keep container tightly closed.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

#### **Hazard statements**

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H319 Causes serious eye irritation  
H317 May cause an allergic skin reaction  
H315 Causes skin irritation  
H302 Harmful if swallowed  
H226 Flammable liquid and vapour

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## 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 : C<sub>15</sub>H<sub>32</sub>N<sub>3</sub>OP  
MW : 301.41

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## 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

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Dry powder Dry sand

#### Unsuitable extinguishing media

Do NOT use water jet.

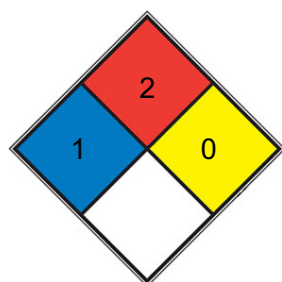
### Special hazards arising from the substance or mixture

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



■ HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

□ SPEC.

□ HAZ.

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## 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.

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# 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.

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# 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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	light yellow viscous
Odour	No data available
Odour Threshold	No data available
pH	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 limits	No data available
Vapour pressure	< 0.1 hPa at 25 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	0.949 g/cm <sup>3</sup> 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

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## 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

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# 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.

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## 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.

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## 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.

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## 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

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## 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

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/>

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

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

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】 ChemIDplus, 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](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.