

SAFETY DATA SHEET

Version 6.15
Revision Date 09/07/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Phosphazene base P₄-*t*-Bu solution

Product Number : 79421
Brand : Aldrich

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Nervous system, H372

Aspiration hazard (Category 1), H304

Short-term (acute) aquatic hazard (Category 3), H402

Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H314	Causes severe skin burns and eye damage.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H372	Causes damage to organs (Nervous system) through prolonged or repeated exposure if inhaled.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.

P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Molecular weight : 633.72 g/mol

Component		Classification	Concentration
Phosphazene base P(4)-tert-butyl			
CAS-No.	111324-04-0	Skin Corr. 1B; Eye Dam. 1; H314, H318	>= 70 - < 90 %
EC-No.	629-524-3		
n-Hexane			
CAS-No.	110-54-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 1; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H361, H336, H372, H304, H401, H411 Concentration limits: >= 5 %: STOT RE 2, H373; >= 20 %: STOT SE 3, H336;	>= 20 - < 30 %
EC-No.	203-777-6		
Index-No.	601-037-00-0		
Registration number	01-2119480412-44-XXXX		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of 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. Call in physician.

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. Immediately call in ophthalmologist.
Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Pulmonary failure possible after aspiration of vomit. Call a physician immediately. Do not attempt to neutralise.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures**5.1 Extinguishing media****Suitable extinguishing media**

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Oxides of phosphorus

Mixture with combustible ingredients.

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.

5.3 Advice for firefighters

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

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures**6.1 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.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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 (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

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

Advice on protection against fire and explosion

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

Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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

Moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
n-Hexane	110-54-3	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		

		TWA	50 ppm 180 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	500 ppm 1,800 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	50 ppm 180 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
n-Hexane	110-54-3	2,5-Hexanedione	0.5 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 30 min

Material tested: Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist

and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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.

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid, clear Color: light yellow
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	No data available
g) Flash point	-26 °C (-15 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.850 - 0.875 g/cm ³ at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	No data available

- o) Partition coefficient: No data available
n-octanol/water
- p) Autoignition No data available
temperature
- q) Decomposition No data available
temperature
- r) Viscosity No data available
- s) Explosive properties Not classified as explosive.
- t) Oxidizing properties none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Inhalation: No data available

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

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

Skin corrosion/irritation

Remarks: Causes skin burns.

Serious eye damage/eye irritation

Remarks: Causes eye burns.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Remarks: No data available

Mixture causes damage to organs through prolonged or repeated exposure.

- Nervous system

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

Warning: contains n-hexane (CAS#110-54-3) a suspected neurotoxin., Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, chest pain, Difficulty in breathing, Lung irritation, Gastrointestinal disturbance, Prolonged or repeated contact with skin may cause:, defatting, Dermatitis, Contact with eyes can cause:, Redness, Blurred vision, Provokes tears., Effects due to ingestion may include:, Gastrointestinal discomfort, Central nervous system depression
Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components

Phosphazene base P(4)-tert-butyl

Acute toxicity

Oral: No data available
Inhalation: No data available
Dermal: No data available
No data available

Skin corrosion/irritation

Remarks: Causes skin burns.

Serious eye damage/eye irritation

Remarks: Causes eye burns.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available
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

n-Hexane

Acute toxicity

LD50 Oral - Rat - male and female - 16,000 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - 4 h - 172 mg/l - vapor
Remarks: (RTECS)
LD50 Dermal - Rabbit - male - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit
Result: Skin irritation - 24 h
(OECD Test Guideline 404)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 478

Species: Mouse - male

Result: negative

Method: OECD Test Guideline 475

Species: Rat - male and female - Bone marrow

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

Inhalation - Causes damage to organs through prolonged or repeated exposure.

- Nervous system

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

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

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

Phosphazene base P(4)-tert-butyl

No data available

n-Hexane

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 2.5 mg/l - 96 h Remarks: (ECOTOX Database)
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Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 2.1 mg/l - 48 h Remarks: (Lit.)
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SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

UN number: 2924 Class: 3 (8) Packing group: II
Proper shipping name: Flammable liquids, corrosive, n.o.s. (n-Hexane, Phosphazene base P(4)-tert-butyl)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2924 Class: 3 (8) Packing group: II EMS-No: F-E, S-C

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Proper shipping name: FLAMMABLE LIQUID, CORROSIVE, N.O.S. (n-Hexane, Phosphazene base P(4)-tert-butyl)

IATA

UN number: 2924 Class: 3 (8)

Packing group: II

Proper shipping name: Flammable liquid, corrosive, n.o.s. (n-Hexane, Phosphazene base P(4)-tert-butyl)

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards

: Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313

: The following components are subject to reporting levels established by SARA Title III, Section 313:

n-Hexane 110-54-3 >= 20 - < 30 %

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

n-Hexane 110-54-3 >= 20 - < 30 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

n-Hexane

110-54-3

Pennsylvania Right To Know

n-Hexane

110-54-3

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

California Prop. 65

WARNING: This product can expose you to chemicals including n-Hexane, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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