



MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 08/21/2013

Version 2.0

SECTION 1. Identification

Product identifier

Product number	843942
Product name	Propanephosphonic acid anhydride (50% solution in ethyl acetate) for synthesis T3P®

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

Identified uses	Use restricted under TSCA to research and development or as analytical reagent. Uses regulated under FDA or FIFRA are not affected. Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America SDS Phone Support: +1-978-715-1335 General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 2, H225
Skin corrosion, Category 1B, H314
Specific target organ systemic toxicity - single exposure, Category 3, H336
For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms



Signal Word
Danger

Hazard Statements

H225 Highly flammable liquid and vapor.

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H314 Causes severe skin burns and eye damage.
H336 May cause drowsiness or dizziness.

Precautionary Statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Chemical nature Mixture of organic compounds

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

ethyl acetate (>= 30 % - < 50 %)

141-78-6

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane (>= 30 % - < 50 %)

68957-94-8

dipropyldiphosphonic acid (>= 10 % - < 30 %)

71760-04-8

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Call in physician.

Skin contact

After skin contact: wash off with plenty of water. Immediately remove contaminated clothing. If available swab with polyethylene glycol 400. Call a physician immediately.

Eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

Ingestion

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

Never give anything by mouth to an unconscious person.

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Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Cough, respiratory paralysis, Shortness of breath, Drowsiness, narcosis, Nausea, Vomiting, Headache, drowsiness

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

Water, Foam

Special hazards arising from the substance or mixture

Combustible material

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

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

Fire may cause evolution of:

Oxides of phosphorus

May not get in touch with:

Water

Caution! in contact with water product releases:

Organic acids

Advice for firefighters

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.

Further information

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

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

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Observe possible material restrictions (see sections 7 and 10).
Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

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

Observe label precautions.

Advice on protection against fire and explosion

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

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store at +2°C to +8°C (+36°F to +46°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>ethyl acetate</i> 141-78-6			
ACGIH	Time Weighted Average (TWA):	400 ppm	
NIOSH/GUIDE	Recommended exposure limit (REL):	400 ppm 1,400 mg/m ³	
OSHA_TRANS	PEL:	400 ppm 1,400 mg/m ³	
Z1A	Time Weighted Average (TWA):	400 ppm 1,400 mg/m ³	

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

Eye/face protection

Tightly fitting safety goggles

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Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

Flame retardant antistatic protective clothing

Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless to light yellow
Odor	No strong odor known.
Odor Threshold	No information available.
pH	No information available.
Melting point	No information available.
Boiling point/boiling range	171 °F (77 °C) at 1,013 hPa ethyl acetate
Flash point	25 °F (-4 °C) Method: c.c. ethyl acetate
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	2.1 %(V) ethyl acetate
Upper explosion limit	11.5 %(V) ethyl acetate
Vapor pressure	97 hPa at 68 °F (20 °C) ethyl acetate

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Relative vapor density	No information available.
Relative density	1.08 g/cm ³ at 68 °F (20 °C)
Water solubility	Hydrolyzis
Partition coefficient: n-octanol/water	No information available.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.

SECTION 10. Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

sensitive to moisture

Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapors with:

Exothermic reaction with:

Fluorine, chlorosulfonic acid, Strong oxidizing agents

Risk of explosion with:

lithium aluminum hydride, Alkali metals, hydrides, fuming sulfuric acid

Violent reactions possible with:

Water

Conditions to avoid

Warming.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Exposure to moisture.

Incompatible materials

no information available

Hazardous decomposition products

in the event of fire: See section 5.

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SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Target Organs

Eyes

Skin

Respiratory system

Acute oral toxicity

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach., Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

Acute inhalation toxicity

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

Skin irritation

Mixture causes burns.

Eye irritation

Mixture causes serious eye damage.

Specific target organ systemic toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
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.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

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Product name

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Quantitative data on the toxicity of this product are not available.

Further toxicological data:

Decomposition of the substance with tissue moisture.

Property that must be anticipated on the basis from the components of the mixture:

Systemic effects:

Nausea, Vomiting, Headache, respiratory paralysis, narcosis, lack of appetite

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Ingredients

ethyl acetate

Acute oral toxicity

LD50 rat: 5,620 mg/kg (RTECS)

Acute inhalation toxicity

LC50 rat: 5.86 mg/l; 8 h (Lit.)

Acute dermal toxicity

LD50 rabbit: > 18,000 mg/kg (External MSDS)

Skin irritation

rabbit

Result: No skin irritation

(IUCLID)

Eye irritation

rabbit

Result: slight irritation

OECD Test Guideline 405

Sensitization

Maximization Test guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Mutagenicity (mammal cell test): chromosome aberration.

Result: negative

(National Toxicology Program)

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane

Acute oral toxicity

LD50 rat: > 2,000 mg/kg (External MSDS)

Acute dermal toxicity

LD50 rat: > 2,000 mg/kg (External MSDS)

Repeated dose toxicity

rat

Oral

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28 d

NOAEL: 62.5 mg/kg
(External MSDS)

dipropyldiphosphonic acid

No information available.

SECTION 12. Ecological information

Ecotoxicity

No information available.

Persistence and degradability

No information available.

Bioaccumulative potential

No information available.

Mobility in soil

No information available.

Ingredients

ethyl acetate

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 230 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 717 mg/l; 48 h (IUCLID)

Toxicity to algae

IC50 Desmodesmus subspicatus (green algae): 3,300 mg/l; 48 h (IUCLID)

Toxicity to bacteria

EC10 Pseudomonas putida: 2,900 mg/l; 16 h (IUCLID)

Biodegradability

100 %; 28 d

OECD Test Guideline 301D

Readily biodegradable.

Theoretical oxygen demand (ThOD)

1,820 mg/g

(Lit.)

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

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane

Toxicity to fish

LC50 Danio rerio (zebra fish): > 100 mg/l; 96 h (External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): > 100 mg/l; 48 h (External MSDS)

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Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): > 100 mg/l; 72 h (External MSDS)

Toxicity to bacteria

IC50 Bacteria: > 1,000 mg/l; 3 h (External MSDS)

Biodegradability

1.9 %; 28 d

OECD Test Guideline 301A

Not readily biodegradable.

Partition coefficient: n-octanol/water

log Pow: 0.49

(External MSDS)

dipropyldiphosphonic acid

No information available.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 2924
Proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S. (CONT. ETHYL ACETATE, PROPYLPHOSPHONIC CYCLIC ANHYDRIDE)
Class	3 (8)
Packing group	II
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 2924
Proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S. (CONT. ETHYL ACETATE, PROPYLPHOSPHONIC CYCLIC ANHYDRIDE)
Class	3 (8)
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

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UN number UN 2924
Proper shipping name FLAMMABLE LIQUID, CORROSIVE, N.O.S. (CONT. ETHYL ACETATE, PROPYLPHOSPHONIC CYCLIC ANHYDRIDE)
Class 3 (8)
Packing group II
Environmentally hazardous --
Special precautions for user yes
EmS F-E S-C
Segregation Group 0001 Acids

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Flammable Liquid
Target organ effects
Corrosive to eyes
Corrosive by inhalation.

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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.

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

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Ingredients

ethyl acetate

Pennsylvania Right To Know

Ingredients

ethyl acetate

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane

dipropyldiphosphonic acid

New Jersey Right To Know

Ingredients

ethyl acetate

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane

dipropyldiphosphonic acid

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.

Ingredients

2,4,6-tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane

dipropyldiphosphonic acid

propylphosphonic acid

DSL: This product contains one or several components that are not on the Canadian DSL nor NDSL.

Ingredients

dipropyldiphosphonic acid

propylphosphonic acid

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Full text of H-Statements referred to under sections 2 and 3.

H225 Highly flammable liquid and vapor.
H314 Causes severe skin burns and eye damage.
H336 May cause drowsiness or dizziness.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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