

Safety Data Sheet

According to EC Directive 91/155/EEC

Date of issue:

17.12.2004

1. Identification of the substance/preparation and of the company/undertaking

Identification of the product

Catalogue No.: 821118
Product name: Thiophosphoryl chloride for synthesis

Use of the substance/preparation

Chemical for synthesis

Company/undertaking identification

Company: Merck Schuchardt OHG * 85662 Hohenbrunn * Germany *
Tel: +49 8102/802-0
Emergency telephone No.: Please contact the regional Merck representation
in your country.

2. Composition/information on ingredients

CAS-No.: 3982-91-0
M: 169.40 g/mol
Formula Hill: Cl₃PS
EC-No.: 223-622-6

3. Hazards identification

Harmful if swallowed. Very toxic by inhalation. Causes burns. Irritating to respiratory system.

4. First aid measures

First-aid personnel: ensure self-protection!

After inhalation: fresh air. Call in physician.

After skin contact: wash off with plenty of water. Dab with polyethylene glycol 400.
Immediately remove contaminated clothing.

After eye contact: rinse out with plenty of water for at least 10 minutes with the eyelid held wide open. Immediately call in ophthalmologist.

After swallowing: make victim drink plenty of water (if necessary several litres), avoid vomiting (risk of perforation!). Immediately call in physician. Do not attempt to neutralize.

Merck Safety Data Sheet

According to EC Directive 91/155/EEC

Catalogue No.: 821118
Product name: Thiophosphoryl chloride for synthesis

5. Fire-fighting measures

Suitable extinguishing media:
CO₂, powder.

Extinguishing media not to be used:
Water, foam.

Special risks:
Development of hazardous combustion gases or vapours possible in the event of fire. The following may develop in event of fire: phosphorus oxides, sulfur oxides, hydrochloric acid.

Caution! in contact with water product releases: corrosive vapours.

Special protective equipment for fire fighting:
Do not stay in dangerous zone without self-contained breathing apparatus. In order to avoid contact with skin, keep a safety distance and wear suitable protective clothing.

Other information:
Non-combustible.

6. Accidental release measures

Person-related precautionary measures:
Avoid substance contact. Do not inhale vapours/aerosols. Ensure supply of fresh air in enclosed rooms.

Environmental-protection measures:
Do not allow to enter sewerage system.

Procedures for cleaning / absorption:
Take up with liquid-absorbent material (e.g. Chemizorb®). Forward for disposal. Clean up affected area.

7. Handling and storage

Handling:

Notes for safe handling:
Work under hood. Do not inhale substance. Avoid generation of vapours/aerosols.
Keep workplace dry. Do not allow product to come into contact with water.

Storage:

Tightly closed in a well-ventilated place. Accessible only for authorised persons. Storage temperature: no restrictions.

8. Exposure controls/personal protection

Personal protective equipment:

Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled. The resistance of the protective clothing to chemicals should be ascertained with the respective supplier.

Respiratory protection: required when vapours/aerosols are generated.

Eye protection: required

Hand protection: required

Merck Safety Data Sheet

According to EC Directive 91/155/EEC

Catalogue No.: 821118
Product name: Thiophosphoryl chloride for synthesis

Other protective equipment: Acid-resistant protective clothing.

Industrial hygiene:
Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Under no circumstances eat or drink at workplace. Work under hood . Do not inhale substance.

9. Physical and chemical properties

Form:	liquid		
Colour:	colourless		
Odour:	pungent		
pH value		not available	
Melting point		-35	°C
Boiling point		125	°C
Ignition temperature		not available	
Flash point		not available	
Explosion limits	lower	not available	
	upper	not available	
Vapour pressure	(25 °C)	29	hPa
Density	(20 °C)	1.63	g/cm ³
Solubility in water	(20 °C)	(decomposition)	
log Pow:		1.85	(calculated)

10. Stability and reactivity

Conditions to be avoided

Moisture.

Substances to be avoided

water.

Hazardous decomposition products

in the event of fire: See chapter 5.

Further information

sensitive to moisture.

11. Toxicological information

Acute toxicity

LC₅₀ (inhalation, rat): 0.14 mg/l /4 h.

LD₅₀ (oral, rat): 750 mg/kg.

Specific symptoms in animal studies:

Skin irritation test: burns.

Merck Safety Data Sheet

According to EC Directive 91/155/EEC

Catalogue No.: 821118
Product name: Thiophosphoryl chloride for synthesis

Subacute to chronic toxicity

Mutagenicity (mammal cell test): chromosome aberration negative.

Further toxicological information

Decomposition of the substance with tissue moisture. After inhalation: Irritations of the mucous membranes, coughing, and dyspnoea.

After skin contact: Burns.

After eye contact: Burns.

After swallowing: burns in mouth, throat, oesophagus and gastrointestinal tract.

Further data

Further hazardous properties cannot be excluded. The product should be handled with the care usual when dealing with chemicals.

12. Ecological information

Biologic degradation:

Hydrolysis leads to formation of: hydrochloric acid.

The following applies to HCl in general: Harmful effect on aquatic organisms. Harmful effect due to pH shift. Biological effects: hydrochloric acid (including such due to reaction): lethal for fish as from 25 mg/l; *Leuciscus idus* LC₅₀: 862 mg/l (1N-solution). Harmful effects begin at: plants 6 mg/l. Does not cause biological oxygen deficit.

Behavior in environmental compartments:

Distribution: log p(o/w): 1.85 (calculated)

No appreciable bioaccumulation potential is to be expected (log P(o/w) 1-3).

Ecotoxic effects:

Fish toxicity: *Danio rerio* LC₅₀: 99 mg/l /96 h

Bacterial toxicity: activated sludge EC₅₀: ~10000 mg/l /3 h

Further ecologic data:

Do not allow to enter waters, waste water, or soil!

13. Disposal considerations

Product:

Chemicals must be disposed of in compliance with the respective national regulations. Under www.retrologistik.de you will find country- and substance-specific information as well as contact partners.

Packaging:

Merck product packaging must be disposed of in compliance with the country-specific regulations or must be passed to a packaging return system. Under www.retrologistik.de you will find special information on the respective national conditions as well as contact partners.

Merck Safety Data Sheet

According to EC Directive 91/155/EEC

Catalogue No.: 821118
Product name: Thiophosphoryl chloride for synthesis

14. Transport information

Road & Rail ADR, RID
UN 1837 THIOPHOSPHORYLCHLORID, 8, II

Inland waterway ADN, ADNR not tested

Sea IMDG-Code
UN 1837 THIOPHOSPHORYL CHLORIDE, 8, II
Ems F-A S-B

Air
THIOPHOSPHORYL CHLORIDE
CAO 8, UN 1837, II
PAX 8, UN 1837, II prohibited

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

15. Regulatory information

Labelling according to EC Directives

Symbol:	T+	Very toxic
R-phrases:	22-26-34-37	Harmful if swallowed. Very toxic by inhalation. Causes burns. Irritating to respiratory system.
S-phrases:	26-28-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Reduced labelling (1999/45/EC, Art. 10,4)

Symbol:	T+	Very toxic
R-phrases:	22-26-34	Harmful if swallowed. Very toxic by inhalation. Causes burns.
S-phrases:	26-28-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

16. Other information

Regional representation:

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to the appropriate safety precautions. It does not represent a guarantee of the properties of the product.