

according to Regulation (EC) No. 1907/2006

Date of issue: 29.04.2015 Version 1.0

#### SECTION 1. Identification of the substance/mixture and of the company/undertaking

#### 1.1 Product identifier

Catalogue No. 808154

Product name Thionyl chloride for synthesis

REACH Registration Number A registration number is not available for this substance as the

substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a

later registration deadline.

CAS-No. 7719-09-7

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

Identified uses Chemical for synthesis

For additional information on uses please refer to the Merck Chemicals

portal (www.merckgroup.com).

# 1.3 Details of the supplier of the safety data sheet

Company Merck KGaA \* 64271 Darmstadt \*Germany\* Telefon:+49 6151 72-0

Responsible Department LS-QHC \* e-mail: prodsafe@merckgroup.com

Regional representation Merck Sdn. Bhd. (Co. No: 178145), No. 4, Jalan U1/26, Section U1,

Hicom Glenmarie Industrial Park, 40150 Shah Alam, Selangor. Tel:

03-74943688 Fax: 03-74910850

1.4 Emergency telephone

number

Customer Call Centre: + 62 0800 140 1253 (Toll Free)

#### **SECTION 2. Hazards identification**

# 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302 Acute toxicity, Category 3, Inhalation, H331

Skin corrosion, Category 1A, H314

Specific target organ toxicity - single exposure, Category 3, H335

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

#### Classification (67/548/EEC or 1999/45/EC)

R14

R29

XnHarmfulR20/22CCorrosiveR35

For the full text of the R-phrases mentioned in this Section, see Section 16.

Catalogue No. 808154

Product name Thionyl chloride for synthesis

#### 2.2 Label elements

# Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms







# Signal word

Danger

#### Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H331 Toxic if inhaled.

H335 May cause respiratory irritation.

EUH014 Reacts violently with water.

EUH029 Contact with water liberates toxic gas.

#### Precautionary statements

Prevention

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

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

#### Reduced labelling (≤125 ml)

Hazard pictograms







#### Signal word Danger

#### Hazard statements

H314 Causes severe skin burns and eye damage.

H331 Toxic if inhaled.

EUH014 Reacts violently with water.

EUH029 Contact with water liberates toxic gas.

#### Precautionary statements

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

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 7719-09-7

# 2.3 Other hazards

None known.

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

#### SECTION 3. Composition/information on ingredients

#### 3.1 Substance

Formula SOCl<sub>2</sub> Cl<sub>2</sub>OS (Hill)

EC-No. 231-748-8 Molar mass 118.97 g/mol

# Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No. Registration number Classification

Thionylchlorid (<= 100 %)

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

7719-09-7 \*)

Acute toxicity, Category 4, H302 Acute toxicity, Category 3, H331 Skin corrosion, Category 1A, H314

Specific target organ toxicity - single exposure, Category 3, H335

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

#### Hazardous components (1999/45/EC)

Chemical Name (Concentration)
CAS-No. Classification
Thionylchlorid (<= 100 %)

7719-09-7 R14

R29

Xn, Harmful; R20/22 C, Corrosive; R35

For the full text of the R-phrases mentioned in this Section, see Section 16.

#### 3.2 Mixture

Not applicable

#### **SECTION 4. First aid measures**

# 4.1 Description of first aid measures

After inhalation: fresh air. If breathing stops: immediately apply artificial respiration, if necessary oxygen. Immediately call in physician.

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

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

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

# 4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Cough, Shortness of breath, Vomiting, Circulatory collapse Risk of corneal clouding.

<sup>\*)</sup> A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

# 4.3 Indication of any immediate medical attention and special treatment needed

No information available.

# **SECTION 5. Firefighting measures**

# 5.1 Extinguishing media

Suitable extinguishing media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media

Water, Foam

# 5.2 Special hazards arising from the substance or mixture

Not combustible.

May not get in touch with:

Water

Caution! in contact with water product releases:

Hydrogen chloride gas, Sulphur oxides

Ambient fire may liberate hazardous vapours.

Fire may cause evolution of:

Chlorine, Sulphur oxides

# 5.3 Advice for firefighters

Special protective equipment 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.

Further information

Suppress (knock down) gases/vapours/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 vapours, 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.

#### 6.2 Environmental precautions

Do not empty into drains.

#### 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

#### 6.4 Reference to other sections

Indications about waste treatment see section 13.

# SECTION 7. Handling and storage

#### 7.1 Precautions for safe handling

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

Advice on safe handling

Observe label precautions.

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

Hygiene measures

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

#### 7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Dry. Tightly closed.

Recommended storage temperature see product label.

# 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

Thionylchlorid (7719-09-7)

MY OEL Ceiling Limit Value:

1 ppm 4.9 mg/m<sup>3</sup>

#### 8.2 Exposure controls

# **Engineering measures**

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

See section 7.1.

# Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material: Viton (R)
Glove thickness: 0.70 mm
Break through time: > 480 min

splash contact:

Glove material: butyl-rubber
Glove thickness: 0.7 mm
Break through time: > 120 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 890 Vitoject® (full contact), KCL 898 Butoject® (splash contact).

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet<(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment
Acid-resistant protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter B (acc. to DIN 3181) for inorganic gases and vapours The entrepeneur 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.

# Environmental exposure controls

Do not empty into drains.

# SECTION 9. Physical and chemical properties

# 9.1 Information on basic physical and chemical properties

Form liquid

Colour yellow

Odour stinging

Odour Threshold No information available.

pH Not applicable

Melting point -104.5 °C

Boiling point/boiling range 76 °C

at 1,013 hPa

Flash point Not applicable

Evaporation rate No information available.

Flammability (solid, gas) No information available.

Lower explosion limit Not applicable

Upper explosion limit Not applicable

Vapour pressure 121 hPa

at 20 °C

Relative vapour density 4.1

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

Density 1.64 g/cm<sup>3</sup>

at 20 °C

Relative density No information available.

Water solubility at 20 °C

(rigorous decomposition)

Partition coefficient: n-

octanol/water Not applicable

Auto-ignition temperature No information available.

Decomposition temperature > 140 °C

Viscosity, dynamic 0.6 mPa.s

at 25 °C

Explosive properties No information available.

Oxidizing properties No information available.

9.2 Other data

Ignition temperature Not applicable

# SECTION 10. Stability and reactivity

# 10.1 Reactivity

See section 10.3

# 10.2 Chemical stability

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

# 10.3 Possibility of hazardous reactions

Generates dangerous gases or fumes in contact with:

Water, Alcohols, bases, acids

Risk of explosion with:

Ammonia, formaldehyde, sulfoxides

Esters, with

Zinc

Esters, with

Iron

Violent reactions possible with:

sodium, Fluorine

# 10.4 Conditions to avoid

Strong heating.

Moisture.

Exposure to moisture

# 10.5 Incompatible materials

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

Metals

# 10.6 Hazardous decomposition products

in the event of fire: See section 5.

# **SECTION 11. Toxicological information**

# 11.1 Information on toxicological effects

Acute oral toxicity LD50 Rat: 324 mg/kg

(IUCLID)

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

absorption

Acute inhalation toxicity LC50 Rat: 2.7 mg/l; 4 h OECD Test Guideline 403 (IUCLID)

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

Acute dermal toxicity

This information is not available.

Skin irritation

Result: Causes burns.

(IUCLID)

Causes poorly healing wounds.

Causes severe burns.

Eye irritation

Result: Causes burns.

(IUCLID)

Risk of corneal clouding. Risk of blindness!

Mixture causes serious eye damage.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

May cause respiratory irritation.

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

# 11.2 Further information

Further toxicological data:

Decomposition of the substance with tissue moisture.

Systemic effects:

After absorption of large quantities:

Vomiting, Lung oedema, Circulatory collapse

Further data:

Handle in accordance with good industrial hygiene and safety practice.

# **SECTION 12. Ecological information**

# 12.1 Toxicity

Toxicity to fish

LC0 Danio rerio (zebra fish): 575 mg/l; 96 h

(IUCLID)

Toxicity to daphnia and other aquatic invertebrates EC0 Daphnia magna (Water flea): 1,150 mg/l; 24 h

(IUCLID)

Toxicity to bacteria

EC50 activated sludge: 3,462 mg/l; 3 h

ISO 8192 (IUCLID)

# 12.2 Persistence and degradability

No information available.

#### 12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

Not applicable

#### 12.4 Mobility in soil

No information available.

#### 12.5 Results of PBT and vPvB assessment

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

# 12.6 Other adverse effects

Additional ecological information

Biological effects:

After hydrolysis acid effect on fish and plankton. Forms corrosive mixtures with water even if diluted. Harmful effect due to pH shift.

Further information on ecology

Discharge into the environment must be avoided.

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

# **SECTION 13. Disposal considerations**

Waste treatment methods

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.

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

According to Quality Environment Regulation (Scheduled Waste) 2005, waste need to be sent to designated premise for recycle, treatment or disposal. Please contact Kualiti Alam for waste classification and correct disposal method.

#### **SECTION 14. Transport information**

Land transport (ADR/RID)

**14.1 UN number** UN 1836

14.2 Proper shipping name THIONYL CHLORIDE

14.3 Class
14.4 Packing group
14.5 Environmentally hazardous
14.6 Special precautions for
yes

user

Tunnel restriction code E

# Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

**14.1 UN number** UN 1836

14.2 Proper shipping name THIONYL CHLORIDE

**14.3 Class** 8

14.4 Packing group

14.5 Environmentally hazardous --14.6 Special precautions for yes

user Not permitted for transport

Sea transport (IMDG)

**14.1 UN number** UN 1836

**14.2 Proper shipping name** THIONYL CHLORIDE

14.3 Class814.4 Packing groupI14.5 Environmentally hazardous--14.6 Special precautions foryes

user

EmS F-A S-B

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

# 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

# **SECTION 15. Regulatory information**

# 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National legislation

Storage class 6.1 D

# 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

# **SECTION 16. Other information**

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

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H331 Toxic if inhaled.

H335 May cause respiratory irritation.

# Full text of R-phrases referred to under sections 2 and 3

R14 Reacts violently with water.

R20/22 Harmful by inhalation and if swallowed.
R29 Contact with water liberates toxic gas.

R35 Causes severe burns.

#### Training advice

Provide adequate information, instruction and training for operators.

#### Labelling

Hazard pictograms





# Signal word Danger

# Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H331 Toxic if inhaled.

H335 May cause respiratory irritation.

EUH014 Reacts violently with water.

EUH029 Contact with water liberates toxic gas.

#### Precautionary statements

Prevention

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

Response

according to Regulation (EC) No. 1907/2006

Catalogue No. 808154

Product name Thionyl chloride for synthesis

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

# Labelling (67/548/EEC or 1999/45/EC)

Symbol(s)	C	Corrosive
R-phrase(s)	14-20/22-29-35	Reacts violently with water. Harmful by inhalation and if swallowed. Contact with water liberates toxic gas. Causes severe burns.
S-phrase(s)	26-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. 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).
EO NI	004 740 0	

EC-No. 231-748-8

Reduced label<u>ling</u> (≤125 ml)

Symbol(s) C Corrosive

R-phrase(s) 20/22-35 S-phrase(s) 26-36/37/39-45 Harmful by inhalation and if swallowed. Causes severe burns. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. 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).

# 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.

# Regional representation

Merck Sdn. Bhd. (Co. No: 178145), No. 4, Jalan U1/26, Section U1, Hicom Glenmarie Industrial Park, 40150 Shah Alam, Selangor. Tel: 03-74943688 Fax: 03-74910850

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