SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers
Product name: 2,4,6-Trichlorophenol for synthesis

<table>
<thead>
<tr>
<th>Product Number</th>
<th>Catalogue No.</th>
<th>Brand</th>
<th>Index-No.</th>
<th>REACH No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.18469</td>
<td>818469</td>
<td>Millipore</td>
<td>604-018-00-5</td>
<td>A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.</td>
</tr>
</tbody>
</table>

CAS-No. : 88-06-2

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified uses: Chemical for synthesis

1.3 Details of the supplier of the safety data sheet
Company: Merck KGaA
Frankfurter Str. 250
D-64271 DARMSTADT

Telephone : +49 (0)6151 72-0
Fax : +49 6151 727780
E-mail address : TechnischerService@merckgroup.com

1.4 Emergency telephone
Emergency Phone # : Werkfeuerwehr: +49 (0)6151/722440 *
Telefax: +49 (0)6151/727780 *
Vergiftungs-Informations-Zentrale
Freiburg: 49(0)76119240 *
CHEMTREC Deutschland: 0800 181 7059

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319
Carcinogenicity (Category 2), H351
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410
2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal word: Warning

Hazard statement(s)
H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H351 Suspected of causing cancer.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)
P201 Obtain special instructions before use.
P273 Avoid release to the environment.
P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P302 + P352 IF ON SKIN: Wash with plenty of water.
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 + P313 IF exposed or concerned: Get medical advice/attention.

Supplemental Hazard Statements
none

Reduced Labeling (<= 125 ml)

Pictogram

Signal word: Warning

Hazard statement(s)
H351 Suspected of causing cancer.

Precautionary statement(s)
P201 Obtain special instructions before use.
P308 + P313 IF exposed or concerned: Get medical advice/attention.

Supplemental Hazard Statements
none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula: C6H3Cl3O
Molecular weight: 197.45 g/mol
CAS-No.: 88-06-2
EC-No.: 201-795-9
Index-No.: 604-018-00-5
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
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. Consult a physician.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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
Water 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
Nature of decomposition products not known.
Combustible.
Fire may cause evolution of:
Hydrogen chloride gas
Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating. Development of hazardous combustion gases or vapours possible in the event of fire.

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**
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. 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.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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.

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
Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

Storage class
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

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
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

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). Safety glasses

**Skin protection**
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).
Full contact
- Material: Nitrile rubber
- Minimum layer thickness: 0,11 mm
- Break through time: 480 min
- Material tested: KCL 741 Dermatril® L

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).
Splash contact
- Material: Nitrile rubber
- Minimum layer thickness: 0,11 mm
- Break through time: 480 min
- Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
Recommended Filter type: Filter A-(P3)

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.

**Control of environmental exposure**
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- **Appearance**
  - Form: powder, finecrystalline
  - Color: gray
b) Odor | No data available  

c) Odor Threshold | No data available  

d) pH | No data available  

e) Melting point/freezing point | 65.0 °C  

f) Initial boiling point and boiling range | 246.0 °C  

g) Flash point | 99 °C - closed cup - c.c.  

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) Relative density | No data available  

n) Water solubility | No data available  

o) Partition coefficient: n-octanol/water | No data available  

p) Autoignition temperature | No data available  

q) Decomposition temperature | No data available  

r) Viscosity | Viscosity, kinematic: No data available  
Viscosity, dynamic: No data available  

s) Explosive properties | No data available  

t) Oxidizing properties | No data available  

9.2 Other safety information  
No data available  

SECTION 10: Stability and reactivity  

10.1 Reactivity  
Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.  
The following applies in general to flammable organic substances and mixtures: in  
correspondingly fine distribution, when whirled up a dust explosion potential may generally  
be assumed.  

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

10.3 Possibility of hazardous reactions  
Violent reactions possible with:  
Strong oxidizing agents  
acid halides  
Acid anhydrides
10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 820,0 mg/kg
Remarks: (RTECS)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - 24 h
Remarks: (RTECS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe eye irritation - 24 h
Remarks: (RTECS)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

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

11.2 Additional Information
Depending on the intensity and duration of exposure, effects may vary from mild irritation to severe destruction of tissue., Damage to the eyes., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Damage to the eyes. -
SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish

LC50 - Lepomis macrochirus (Bluegill sunfish) - 0.32 mg/l - 96 h
Remarks: (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 2.2 mg/l - 48 h
Remarks: (ECOTOX Database)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

Bioaccumulation

Poecilia reticulata (guppy) - 36 d
- 0.0005 mg/l(2,4,6,-Trichlorophenol)

Bioconcentration factor (BCF): 12.180

Bioaccumulation

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Other adverse effects

No data available

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions. Notice Directive on waste 2008/98/EC.

SECTION 14: Transport information

14.1 UN number


14.2 UN proper shipping name

ADR/RID: CHLOROPHENOLS, SOLID
IMDG: CHLOROPHENOLS, SOLID
IATA: Chlorophenols, solid

14.3 Transport hazard class(es)

ADR/RID: 6.1  IMDG: 6.1  IATA: 6.1

14.4 Packaging group

ADR/RID: III  IMDG: III  IATA: III
14.5 Environmental hazards
ADR/RID: yes  IMDG Marine pollutant: yes  IATA: no

14.6 Special precautions for user
No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation
Water contaminating class (Germany):
WGK 3, highly water endangering - self classification
Classification according to AwSV, Annex 1 (4)

Other regulations
Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
Take note of Dir 94/33/EC on the protection of young people at work.

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.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H351  Suspected of causing cancer.
H400  Very toxic to aquatic life.
H410  Very toxic to aquatic life with long lasting effects.

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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