SAFETY DATA SHEET

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

1.1 Product identifiers

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

Product Number: 8.18469
Catalogue No.: 818469
Brand: Millipore
CAS-No.: 88-06-2

1.2 Other means of identification

No data available

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

Identified uses: Chemical for synthesis

1.4 Details of the supplier of the safety data sheet

Company: SIGMA-ALDRICH NEW ZEALAND CO.
PO Box 106-406
1143 AUCKLAND
NEW ZEALAND

Telephone: 0800 936 666
Fax: 0800 937 777

1.5 Emergency telephone

Emergency Phone #: 0800 928 888 (NZ)
+64 9 801 0034 (Int'l CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

2.2 GHS Label elements, including precautionary statements

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture: Substance

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.
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

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). 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**
required when dusts 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.

SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a) Appearance</strong></td>
<td>Form: powder, finecrystalline</td>
</tr>
<tr>
<td>Color</td>
<td>gray</td>
</tr>
<tr>
<td><strong>b) Odor</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>c) Odor Threshold</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>d) pH</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>e) Melting point/freezing point</strong></td>
<td>65.0 °C</td>
</tr>
<tr>
<td><strong>f) Initial boiling point and boiling range</strong></td>
<td>246.0 °C</td>
</tr>
<tr>
<td><strong>g) Flash point</strong></td>
<td>99 °C - closed cup - c.c.</td>
</tr>
</tbody>
</table>
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  
   1.675 g/cm³ at 25 °C
   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  
   none

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**
Limited evidence of carcinogenicity in animal studies

**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**
EC50 - Daphnia magna (Water flea) - 2.2 mg/l - 48 h
and other aquatic invertebrates

**12.2 Persistence and degradability**
No data available

**12.3 Bioaccumulative potential**

<table>
<thead>
<tr>
<th>Bioaccumulation</th>
<th>Remarks: (ECOTOX Database)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poecilia reticulata (guppy) - 36 d</td>
<td>0.0005 mg/l(2,4,6,-Trichlorophenol)</td>
</tr>
<tr>
<td>Bioconcentration factor (BCF): 12,180</td>
<td></td>
</tr>
</tbody>
</table>

**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

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

**SECTION 14: Transport information**

**14.1 UN number**

<table>
<thead>
<tr>
<th>ADR/RID</th>
<th>IMDG</th>
<th>IATA-DGR</th>
</tr>
</thead>
<tbody>
<tr>
<td>2020</td>
<td>2020</td>
<td>2020</td>
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</tbody>
</table>

**14.2 UN proper shipping name**

<table>
<thead>
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<th>IATA-DGR</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHLOROPHENOLS, SOLID</td>
<td>CHLOROPHENOLS, SOLID</td>
<td>Chlorophenols, solid</td>
</tr>
</tbody>
</table>

**14.3 Transport hazard class(es)**

<table>
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<th>IMDG</th>
<th>IATA-DGR</th>
</tr>
</thead>
<tbody>
<tr>
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</tbody>
</table>

**14.4 Packaging group**

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<thead>
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<th>IATA-DGR</th>
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</thead>
<tbody>
<tr>
<td>III</td>
<td>III</td>
<td>III</td>
</tr>
</tbody>
</table>

**14.5 Environmental hazards**

<table>
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<th>ADR/RID</th>
<th>IMDG</th>
<th>IATA-DGR</th>
</tr>
</thead>
<tbody>
<tr>
<td>yes</td>
<td>IMDG Marine pollutant: yes</td>
<td>no</td>
</tr>
</tbody>
</table>

**14.6 Special precautions for user**
None

**14.7 Incompatible materials**

**Other regulations**
SECTION 15: Regulatory information

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

National regulatory information
HSNO Approval Code: HSR005155

HSNO Group Standard Approval: not required
Tracking Required: not required
Approved Handler Cert.: not required

Notification status
AICS: On the inventory, or in compliance with the inventory
DSL: None of the components of this product are on the Canadian DSL, but all are on the NDSL
ENCS: On the inventory, or in compliance with the inventory
ISHL: On the inventory, or in compliance with the inventory
KECI: On the inventory, or in compliance with the inventory
NZIoC: On the inventory, or in compliance with the inventory
PICCS: On the inventory, or in compliance with the inventory

SECTION 16: Other information

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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