

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 21.11.2010

Version 4.3

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

1.1 Product identifier

| | |
|---------------------------|--|
| Catalogue No. | 820630 |
| Product name | Hexachloroacetone 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. |

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.merck-chemicals.com). |
|-----------------|---|

1.3 Details of the supplier of the safety data sheet

| | |
|------------------------|---|
| Company | Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0 |
| Responsible Department | LS-QHC * e-mail: prodsafe@merckgroup.com |

| | |
|--------------------------------|---|
| 1.4 Emergency telephone number | Please contact the regional company representation in your country. |
|--------------------------------|---|

2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302

Chronic aquatic toxicity, Category 2, H411

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

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

Xn; R22

N; R51/53

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H302 Harmful if swallowed.

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H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

P273 Avoid release to the environment.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

Index-No. 606-032-00-7

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

| | | |
|--------------|----------|--|
| Symbol(s) | Xn | Harmful |
| | N | Dangerous for the environment |
| R-phrases(s) | 22-51/53 | Harmful if swallowed. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. |
| S-phrases(s) | 24/25-61 | Avoid contact with skin and eyes. Avoid release to the environment. Refer to special instructions/ Safety data sheets. |

EC-No. 204-129-5 EC Label

Reduced labelling (≤125 ml)

| | | |
|--------------|-------|-----------------------------------|
| Symbol(s) | Xn | Harmful |
| | N | Dangerous for the environment |
| R-phrases(s) | 22 | Harmful if swallowed. |
| S-phrases(s) | 24/25 | Avoid contact with skin and eyes. |

2.3 Other hazards

None known.

3. Composition/information on ingredients

| | | |
|------------|-------------------------------------|---|
| Formula | CCl ₃ COCCl ₃ | C ₃ Cl ₆ O (Hill) |
| CAS-No. | 116-16-5 | |
| Index-No. | 606-032-00-7 | |
| EC-No. | 204-129-5 | |
| Molar mass | 264,75 g/mol | |

4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Get medical attention.

After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

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

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

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4.2 Most important symptoms and effects, both acute and delayed
irritant effects, Drowsiness, Dizziness

4.3 Indication of immediate medical attention and special treatment needed
No information available.

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, 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

Combustible material, Vapours are heavier than air and may spread along floors.

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

Fire may cause evolution of:

Hydrogen chloride gas, Phosgene

5.3 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

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

6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapours, aerosols. 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 7.2 and 10.5).

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.

7. Handling and storage

7.1 Precautions for safe handling

Observe label precautions.

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7.2 Conditions for safe storage, including any incompatibilities

Tightly closed.

Store at +15°C to +25°C.

7.3 Specific end uses

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. Exposure controls/personal protection

8.1 Control parameters

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.

Hygiene measures

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

Eye/face protection

Safety glasses

Hand protection

full contact:

| | |
|---------------------|----------------|
| Glove material: | Nitrile rubber |
| Glove thickness: | 0,40 mm |
| Break through time: | > 480 min |

splash contact:

| | |
|---------------------|----------------|
| Glove material: | Nitrile rubber |
| Glove thickness: | 0,11 mm |
| Break through time: | > 30 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 730 Camatril® -Velours (full contact), KCL 741 Dermatril® L (splash contact).

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:

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective

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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.

9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

| | |
|--|--|
| Form | liquid |
| Colour | colourless |
| Odour | stinging |
| Odour Threshold | No information available. |
| pH | No information available. |
| Melting point | -3 °C |
| Boiling point/boiling range | 203 - 205 °C |
| Flash point | No information available. |
| Evaporation rate | No information available. |
| Flammability (solid, gas) | No information available. |
| Lower explosion limit | No information available. |
| Upper explosion limit | No information available. |
| Vapour pressure | No information available. |
| Relative vapour density | No information available. |
| Relative density | 1,74 g/cm ³ at 20 °C |
| Water solubility | at 20 °C slightly soluble |
| Partition coefficient: n-octanol/water | log Pow: 2,48 Method: (calculated) No remarkable bioaccumulation potential is expected (log Pow 1-3). (Lit.) |
| Autoignition temperature | No information available. |
| Decomposition temperature | No information available. |
| Viscosity, dynamic | No information available. |

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| | |
|----------------------|---------------------------|
| Explosive properties | No information available. |
|----------------------|---------------------------|

| | |
|----------------------|---------------------------|
| Oxidizing properties | No information available. |
|----------------------|---------------------------|

9.2 Other data

none

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

Strong oxidizing agents, Bases

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See chapter 5.

11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity
absorption

Acute dermal toxicity
LD50 rabbit
Dose: 2.980 mg/kg
(RTECS)

absorption

Skin irritation
slight irritation

Eye irritation
slight irritation

Specific target organ toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

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

Aspiration hazard
No aspiration toxicity classification

11.2 Further information

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Further information

Systemic effects:

Dizziness, Drowsiness

Damage to:

Kidney, Liver

Further data:

Handle in accordance with good industrial hygiene and safety practice.

12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,48

Method: (calculated)

No remarkable bioaccumulation potential is expected (log Pow 1-3). (Lit.)

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Do not allow to run into surface waters, wastewater, or soil.

13. Disposal considerations

Waste treatment methods

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

14. Transport information

ADR/RID

UN 2661 HEXACHLOROACETONE, 6.1, III

IATA

UN 2661 HEXACHLOROACETONE, 6.1, III

IMDG

UN 2661 HEXACHLOROACETONE, 6.1, III

EmS F-A S-A

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

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

The Safety Data Sheets for catalogue items are available at www.merckgroup.com

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EU regulations

| | |
|-----------------------------------|---|
| Major Accident Hazard Legislation | 96/82/EC Dangerous for the environment 9b Quantity 1: 200 t Quantity 2: 500 t |
|-----------------------------------|---|

| | |
|---------------------------|---|
| Occupational restrictions | Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers. |
|---------------------------|---|

National legislation

| | |
|-------------------|----------------------------------|
| Storage class VCI | 10 - 13 Other liquids and solids |
|-------------------|----------------------------------|

15.2 Chemical Safety Assessment

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

16. Other information

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

| | |
|------|--|
| H302 | Harmful if swallowed. |
| H411 | Toxic to aquatic life with long lasting effects. |

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

| | |
|--------|---|
| R22 | Harmful if swallowed. |
| R51/53 | Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. |

Training advice

Provide adequate information, instruction and training for operators.

| | |
|--------------------------|---|
| Regional representation: | This information is given on the authorised Safety Data Sheet for your country. |
|--------------------------|---|

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.

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.