

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 07.06.2017

Version 6.6

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

### 1.1 Product identifier

Catalogue No. 820647

Product name 4-Hexylresorcinol 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. 136-77-6

### 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](http://www.merckgroup.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](mailto:prodsafe@merckgroup.com)

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

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## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

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Acute toxicity, Category 4, Oral, H302

Skin irritation, Category 2, H315

Eye irritation, Category 2, H319

For the full text of the H-Statements 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.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

*Precautionary statements*

Prevention

P260 Do not breathe vapour.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and 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.

**Reduced labelling ( $\leq 125$  ml)**

*Hazard pictograms*



*Signal word*

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Warning

CAS-No. 136-77-6

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula 4-[CH<sub>3</sub>(CH<sub>2</sub>)<sub>5</sub>]C<sub>6</sub>H<sub>3</sub>-1,3-(OH)<sub>2</sub> C<sub>12</sub>H<sub>18</sub>O<sub>2</sub> (Hill)  
Molar mass 194,27 g/mol

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

*Chemical name (Concentration)*

CAS-No. Registration number Classification

4-Hexylresorcinol (<= 100 % )

136-77-6 \*)

Acute toxicity, Category 4, H302

Skin irritation, Category 2, H315

Eye irritation, Category 2, H319

\*) 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.

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

### 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air.

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In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

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

irritant effects

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

#### *Suitable extinguishing media*

Water, Foam, Carbon dioxide (CO<sub>2</sub>), 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.

Vapours 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

#### *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*

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.

Advice for emergency responders:

Protective equipment 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

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

#### *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*

Protected from light.

Tightly closed. Dry.

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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.

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## SECTION 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.

##### *Eye/face protection*

Safety glasses

##### *Hand protection*

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

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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 741 Dermatril® L (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](http://www.kcl.de)).

#### *Other protective equipment*

protective clothing

#### *Respiratory protection*

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

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.

#### **Environmental exposure controls**

Do not let product enter drains.

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## **SECTION 9. Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

Form	powder, finocrystalline
Colour	light pink
Odour	stinging
Odour Threshold	No information available.

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pH	7,7 at 0,5 g/l 20 °C
Melting point/range	64 - 67 °C
Boiling point/boiling range	333 - 335 °C at 1.013 hPa
Flash point	> 100 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	Not applicable
Upper explosion limit	Not applicable
Vapour pressure	No information available.
Relative vapour density	No information available.
Density	No information available.
Relative density	No information available.
Water solubility	0,5 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,45 (experimental) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.

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Decomposition temperature	> 333 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Bulk density	ca.340 kg/m <sup>3</sup>
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## 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

Sensitivity to light

Sensitive to air.

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, Acid anhydrides, acid halides

### 10.4 Conditions to avoid

Exposure to light.

Strong heating.

### 10.5 Incompatible materials

no information available

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## 10.6 Hazardous decomposition products

no information available

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: 550 mg/kg

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

(External MSDS)

absorption

#### *Acute inhalation toxicity*

Symptoms: Possible damages:, mucosal irritations

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

Causes skin irritation.

#### *Eye irritation*

Causes serious eye irritation.

#### *Sensitisation*

This information is not available.

#### *Germ cell mutagenicity*

#### *Genotoxicity in vitro*

Mutagenicity (mammal cell test):

Result: positive

(National Toxicology Program)

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Ames test  
Salmonella typhimurium  
Result: negative

(National Toxicology Program)  
Mutagenicity (mammal cell test): chromosome aberration.  
Result: negative

(National Toxicology Program)

*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*  
This information is not available.

*Specific target organ toxicity - repeated exposure*  
This information is not available.

*Aspiration hazard*  
This information is not available.

## 11.2 Further information

Handle in accordance with good industrial hygiene and safety practice.  
Other dangerous properties can not be excluded.

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## SECTION 12. Ecological information

### 12.1 Toxicity

No information available.

### 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

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*Partition coefficient: n-octanol/water*

log Pow: 3,45

(experimental)

Bioaccumulation is not expected. (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*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

**Land transport (ADR/RID)**

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

**Inland waterway transport (ADN)**

Not relevant

**Air transport (IATA)**

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

**Sea transport (IMDG)**

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**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

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

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard	SEVESO III
Legislation	Not applicable

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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Substances of very high concern (SVHC)	This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1$ % (w/w).
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#### *National legislation*

Storage class	10 - 13
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### 15.2 Chemical safety assessment

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

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## 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.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*

H302 Harmful if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.

*Precautionary statements*

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and 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.  
P313 Get medical advice/ attention.

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## 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](http://www.wikipedia.org).

## Regional representation

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

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*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.*