

According to Regulation (EC) No 1907/2006

4-Hexylresorcinol



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

1.1. Product identifier

Trade name

4-Hexylresorcinol

CAS number

136-77-6

EC number

205-257-4

Synonyms

4-hexyl-1,3-dihydroxy-benzene

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

Relevant identified uses

Research and development.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Street address

Molekula Ltd, Lingfield Way, Darlington,

DL1 4XX Darlington

United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email address

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Hazardous to the aquatic environment — Chronic hazard category 2

Eye irritation, hazard category 2

Acute toxicity, oral, hazard category 4

Hazard statements

H302, H319, H411

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Warning

Hazard statements

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

P264 Wash thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P273 Avoid release to the environment.

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

P330 Rinse mouth.

P391 Collect spillage.

P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337 + P313 If eye irritation persists: Get medical advice/attention.

P501 Dispose of contents/container to .

2.3. Other hazards

No data available

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SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrases M factor acute M factor chronic	Note
4-Hexylresorcinol	136-77-6 205-257-4 - -	100%	Acute Tox. 4 - oral, Eye Irrit. 2, Aquatic Chronic 2	H302, H319, H411 - -	-

Molecular weight

194.27

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. In case of persistent throat irritation or coughing: Seek medical attention and bring these instructions.

Skin contact

IF ON SKIN: Wash with plenty of water. Continue to rinse for at least 15 minutes and seek medical attention. Get medical advice/attention if you feel unwell.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell.

Information for doctors

First aiders/ medical personnel need to protect themselves.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

Inhalation

Single exposure may cause the following adverse effects: Upper respiratory irritation. Difficulty in breathing.

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Skin contact

Single exposure may cause the following adverse effects: Severe skin irritation.

Eye contact

Single exposure may cause the following adverse effects: Severe irritation.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. Nausea, vomiting.

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

Treat symptomatically. No special treatment requirement.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide or dry powder to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards:

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon dioxide (CO₂).

Carbon monoxide (CO).

Combustible.

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Avoid inhalation of dust and contact with skin and eyes. Provide adequate ventilation. For personal protection, see section 8.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container. Store in closed original container at temperatures between 8°C and 21°C. 35.6-46.4°F

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits

No occupational exposure limit assigned.

8.2. Exposure controls

Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Nitrile gloves are recommended. No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Colour

No data available

Odour

No data available

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Melting point / freezing point

65 - 67 °C - lit.

Boiling point or initial boiling point and boiling range

333 - 335 °C - lit.

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

198 °C

Auto-ignition temperature

ca.450 °C

Decomposition temperature

No data available

pH

No data available

Kinematic viscosity

No data available

Solubility

ca.0.701g/l at 20 °C

Partition coefficient n-octanol/water

log Pow: ca.3.34 at 20 °C

Vapour pressure

No data available

Density and/or relative density

ca.1.036 g/cm³ at 20 °C

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

Surface Tension: 36.59 mN/m at 20 °C

SECTION 10: Stability and reactivity

10.1. Reactivity

Forms explosive mixtures with air.

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10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidising agents.

Acid anhydrides.

10.4. Conditions to avoid

Heating.

10.5. Incompatible materials

No data available

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Test animals
4-Hexylresorcinol 136-77-6 / 205-257-4	Acute Toxicity (Oral LD50):	550 mg/kg	Rat

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	No skin irritation.	Human

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	Causes eye irritation.	Rabbit

Respiratory or skin sensitisation

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Product / Substance name CAS / EC no.	Result	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	Negative.	Mouse

Germ cell mutagenicity

Product / Substance name CAS / EC no.	Result	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	Negative.	Salmonella typhimurium

Carcinogenicity

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

11.2. Information on other hazards

No data available

SECTION 12: Ecological information**12.1. Toxicity****Acute algae toxicity**

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	EC50	6.24m/l	72 hours	Pseudokirchneriella subcapitata

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-Hexylresorcinol 136-77-6 / 205-257-4	EC50	2.8mg/l	48 hours	Daphnia magna

12.2. Persistence and degradability**Persistence and degradability**

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Product / Substance name CAS / EC no.	Duration	Result	Degradation
4-Hexylresorcinol 136-77-6 / 205-257-4	28 days	11.36%	The product is expected to be slowly biodegradable.

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

No data available

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal considerations**

Dispose of contents/container in accordance with international regulations.

SECTION 14: Transport information**14.1. UN number**

3077

14.2. UN proper shipping name**ADR / RID / ADN proper shipping name**

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

IMDG proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

IATA proper shipping name

Environmentally hazardous substance, solid, n.o.s.

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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



9 Environmental hazard

IMDG



9

IATA



9 Environmental hazard

ADR / RID Class

9

ADR / RID Classification code

M7

ADR / RID hazard identification number

90

IMDG Class

9

IATA Class

9

ADN Class

9

ADN Class Code

M7

14.4. Packing group

ADR / RID / ADN: III

IMDG: III

IATA: III

14.5. Environmental hazards

ADR/RID/ADN: Hazardous for the environment

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IMDG EmS

F-A, S-F

14.6. Special precautions for user

Tunnel restriction code: -

Transport category: 3

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

SECTION 15: Regulatory information

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

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National regulations

No data available

15.2. Chemical safety assessment

No data available

SECTION 16: Other information

Phrase meaning

Aquatic Chronic 2 - Hazardous to the aquatic environment — Chronic hazard category 2

Eye Irrit. 2 - Eye irritation, hazard category 2

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.