



SAFETY DATA SHEET

4-Phenyl-1-cyclohexene

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	4-Phenyl-1-cyclohexene
Product number	89988564
CAS number	4994-16-5
EC number	690-147-2

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

Identified uses	For research purposes only.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Not Classified
Environmental hazards	Not Classified

2.2. Label elements

EC number	690-147-2
Hazard statements	NC Not Classified

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	4-Phenyl-1-cyclohexene
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4-Phenyl-1-cyclohexene

CAS number	4994-16-5
EC number	690-147-2
Chemical formula	C ₁₂ H ₁₄

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	If in doubt, get medical attention promptly. Show this Safety Data Sheet to the medical personnel.
Inhalation	No specific recommendations. If throat irritation or coughing persists, proceed as follows. Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if any discomfort continues.
Ingestion	No specific recommendations. If throat irritation or coughing persists, proceed as follows. Rinse mouth. Get medical attention if any discomfort continues.
Skin contact	No specific recommendations. Rinse with water. Get medical attention if any discomfort continues.
Eye contact	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
Protection of first aiders	Use protective equipment appropriate for surrounding materials.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Temporary irritation.
Ingestion	May cause discomfort if swallowed.
Skin contact	May cause discomfort.
Eye contact	May be slightly irritating to eyes.

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

Notes for the doctor	Treat symptomatically.
Specific treatments	No special treatment required.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards	Containers can burst violently or explode when heated, due to excessive pressure build-up.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Carbon dioxide (CO ₂). Carbon monoxide (CO).

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5.3. Advice for firefighters

Protective actions during firefighting	Avoid breathing fire gases or vapours. Evacuate area. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. If a leak or spill has not ignited, use water spray to disperse vapours and protect men stopping the leak.
Special protective equipment for firefighters	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions	No specific recommendations. For personal protection, see Section 8.
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6.2. Environmental precautions

Environmental precautions	Avoid discharge into drains or watercourses or onto the ground.
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6.3. Methods and material for containment and cleaning up

Methods for cleaning up	Reuse or recycle products wherever possible. Absorb spillage to prevent material damage. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dispose of contents/container in accordance with national regulations.
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6.4. Reference to other sections

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

Usage precautions	Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Handle all packages and containers carefully to minimise spills. Keep container tightly sealed when not in use. Avoid the formation of mists.
Advice on general occupational hygiene	Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions	Store away from incompatible materials (see Section 10). No specific recommendations.
Storage class	Unspecified storage.

7.3. Specific end use(s)

Specific end use(s)	The identified uses for this product are detailed in Section 1.2.
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SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

Appropriate engineering controls	No specific ventilation requirements.
Eye/face protection	No specific eye protection required during normal use. Large Spillages: Eyewear complying with an approved standard should be worn if a risk assessment indicates eye contact is possible.
Hand protection	No specific hand protection recommended. Large Spillages: Wear protective gloves.

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Hygiene measures	Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.
Respiratory protection	No specific recommendations. Provide adequate ventilation. Large Spillages: If ventilation is inadequate, suitable respiratory protection must be worn.
Environmental exposure controls	Not regarded as dangerous for the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Colourless liquid.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	-14°C/6.8°F
Initial boiling point and range	235°C/455°F
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	0.97
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	158.24
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
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10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
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10.4. Conditions to avoid

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Conditions to avoid Avoid heat.

10.5. Incompatible materials

Materials to avoid Strong oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended.
Thermal decomposition or combustion products may include the following substances:
Harmful gases or vapours.
Carbon dioxide (CO₂).
Carbon monoxide (CO).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

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

Acute toxicity - dermal

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

Acute toxicity - inhalation

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

Skin corrosion/irritation

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

Serious eye damage/irritation

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

Respiratory sensitisation

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

Skin sensitisation

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

Germ cell mutagenicity

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

Carcinogenicity

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

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

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

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

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

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General information	No specific health hazards known. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Temporary irritation.
Ingestion	May cause discomfort if swallowed.
Skin contact	May cause discomfort.
Eye contact	May be slightly irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

SECTION 12: Ecological information

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.
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12.1. Toxicity

Acute aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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Chronic aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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12.2. Persistence and degradability

Persistence and degradability	The degradability of the product is not known.
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12.3. Bioaccumulative potential

Bioaccumulative potential	No data available on bioaccumulation.
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Partition coefficient	No information available.
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12.4. Mobility in soil

Mobility	No data available.
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12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects	None known.
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SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way.
Disposal methods	Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste packaging should be collected for reuse or recycling. Incineration or landfill should only be considered when recycling is not feasible. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of the local water authority.

SECTION 14: Transport information

General	The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).
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14.1. UN number

Not applicable.

14.2. UN proper shipping name

Not applicable.

14.3. Transport hazard class(es)

No transport warning sign required.

14.4. Packing group

Not applicable.

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78

and the IBC Code

SECTION 15: Regulatory information

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

National regulations

Health and Safety at Work etc. Act 1974 (as amended).

The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment

Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].

EH40/2005 Workplace exposure limits.

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

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**Abbreviations and acronyms
used in the safety data sheet**

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
IATA: International Air Transport Association.
ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
IMDG: International Maritime Dangerous Goods.
CAS: Chemical Abstracts Service.
ATE: Acute Toxicity Estimate.
LC50: Lethal Concentration to 50 % of a test population.
LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).
EC₅₀: 50% of maximal Effective Concentration.
PBT: Persistent, Bioaccumulative and Toxic substance.
vPvB: Very Persistent and Very Bioaccumulative.

Training advice

Only trained personnel should use this material.

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Revision

1

SDS number

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This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.