

## SAFETY DATA SHEET

Version 6.3  
Revision Date 11/08/2021  
Print Date 02/05/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 4'-Pentyl-4-biphenylcarbonitrile

Product Number : 328510  
Brand : Aldrich  
CAS-No. : 40817-08-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Skin sensitization (Category 1), H317

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

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word : Warning

Hazard statement(s)  
H317 : May cause an allergic skin reaction.

Precautionary statement(s)  
P261 : Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

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|             |                                                                      |
|-------------|----------------------------------------------------------------------|
| P272        | Contaminated work clothing must not be allowed out of the workplace. |
| P280        | Wear protective gloves.                                              |
| P302 + P352 | IF ON SKIN: Wash with plenty of soap and water.                      |
| P333 + P313 | If skin irritation or rash occurs: Get medical advice/ attention.    |
| P363        | Wash contaminated clothing before reuse.                             |
| P501        | Dispose of contents/ container to an approved waste disposal plant.  |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                     |
|------------------|-------------------------------------|
| Formula          | : C <sub>18</sub> H <sub>19</sub> N |
| Molecular weight | : 249.35 g/mol                      |
| CAS-No.          | : 40817-08-1                        |
| EC-No.           | : 255-093-2                         |

| Component                              | Classification     | Concentration |
|----------------------------------------|--------------------|---------------|
| <b>4-Cyano-4'-pentyl-1,1'-biphenyl</b> |                    |               |
|                                        | Skin Sens. 1; H317 | <= 100 %      |

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

## 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.

#### 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. 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

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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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

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.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. 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 with liquid-absorbent material (e.g. Chemisorb® ). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

#### **Storage conditions**

Tightly closed.

Hygroscopic.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### 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

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 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

required

##### Body Protection

protective clothing

##### Respiratory protection

required when vapours/aerosols 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.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                                            |                                             |
|--------------------------------------------|---------------------------------------------|
| a) Appearance                              | Form: liquid                                |
| b) Odor                                    | No data available                           |
| c) Odor Threshold                          | No data available                           |
| d) pH                                      | No data available                           |
| e) Melting point/freezing point            | No data available                           |
| f) Initial boiling point and boiling range | 140 - 150 °C 284 - 302 °F at 0.7 hPa - lit. |
| g) Flash point                             | No data available                           |
| 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                                      | 1.008 g/cm <sup>3</sup> at 25 °C (77 °F) - lit. |
|    | Relative density                             | No data available                               |
| n) | Water solubility                             | No data available                               |
| o) | Partition coefficient: n-octanol/water       | log Pow: 5.82 - EPI Suite™                      |
| p) | Autoignition temperature                     | No data available                               |
| q) | Decomposition temperature                    | No data available                               |
| r) | Viscosity                                    | No data available                               |
| s) | Explosive properties                         | No data available                               |
| t) | Oxidizing properties                         | No data available                               |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Avoid moisture.  
no information available

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 4,090 mg/kg

Remarks: (own results)

Inhalation: No data available

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LD50 Dermal - Rat - > 4,000 mg/kg

Remarks: (own results)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation

Remarks: (own results)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

Remarks: (own results)

#### **Respiratory or skin sensitization**

Sensitisation test (Magnusson and Kligman):

Result: positive

Remarks: (own results)

May cause sensitization by skin contact.

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### **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**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Further toxicological data:

Other dangerous properties can not be excluded.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

No data available

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

No data available

### 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

We have no quantitative data concerning the ecological effects of this product.  
Further information on ecology  
Discharge into the environment must be avoided.

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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](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

### DOT (US)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

### Further information

Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Acute Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

4-Cyano-4'-pentyl-1,1'-biphenyl

CAS-No.  
40817-08-1

Revision Date

**New Jersey Right To Know Components**

4-Cyano-4'-pentyl-1,1'-biphenyl

CAS-No.  
40817-08-1

Revision Date

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**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](http://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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