SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 2,4-Hexadienoic acid
Product Number: W392103
Brand: Aldrich
CAS-No.: 110-44-1

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 irritation (Category 2), H315
Eye irritation (Category 2A), H319
Short-term (acute) aquatic hazard (Category 3), H402

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

Aldrich - W392103
Hazard statement(s)
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H402 Harmful to aquatic life.

Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
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.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P362 Take off contaminated clothing and wash 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
Synonyms: Sorbic acid
2,4-Hexadienoic acid

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbic acid</td>
<td>Skin Irrit. 2; Eye Irrit. 2A;</td>
<td>&lt;= 100 %</td>
</tr>
<tr>
<td></td>
<td>Aquatic Acute 3; H315, H319, H402</td>
<td></td>
</tr>
</tbody>
</table>

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.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) 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
Combustible.
Vapors 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
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
Prevent fire extinguishing water from contaminating surface water or the ground water system.

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.
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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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. Dry.

- **Light sensitive.**

- **Storage class**
  Storage class (TRGS 510): 11: Combustible Solids

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**
  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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

  - **Full contact**
  - **Material:** Nitrile rubber
  - **Minimum layer thickness:** 0.11 mm
  - **Break through time:** 480 min

  **Material tested:** KCL 741 Dermatril® L
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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
Recommended Filter type: Filter type P2
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.

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**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: crystalline</td>
</tr>
<tr>
<td></td>
<td>Color: white</td>
</tr>
<tr>
<td>b) Odor</td>
<td>weak</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>3.3 at 1.6 g/l at 20 °C (68 °F)</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: 132 - 135 °C (270 - 275 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>&gt; 160 - &lt; 260 °C &gt; 320 - &lt; 500 °F at 1,013 hPa - OECD Test Guideline 103 - (decomposition)</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>127 °C (261 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
</tbody>
</table>
k) Vapor pressure 0.01 hPa at 20 °C (68 °F)
l) Vapor density 3.87
m) Density 1.2 g/cm³ at 20 °C (68 °F) - OECD Test Guideline 109
   Relative density No data available
n) Water solubility 1.6 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: log Pow: 1.32 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature does not ignite
q) Decomposition temperature > 170 °C (> 338 °F) -
r) Viscosity No data available
s) Explosive properties No data available
t) Oxidizing properties none

9.2 Other safety information
Relative vapor density 3.87

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

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents
Bases

10.4 Conditions to avoid
Light.
Strong heating.

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5
SECTION 11: Toxicological information

11.1 Information on toxicological effects

**Acute toxicity**
LD50 Oral - Rat - male and female - 10,500 mg/kg
Remarks: (ECHA)
Inhalation: No data available
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

**Skin corrosion/irritation**
Remarks: Causes skin irritation.
(ECHA)

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: Eye irritation - 24 h
(OECD Test Guideline 405)

**Respiratory or skin sensitization**
Maximization Test - Guinea pig
Result: negative

**Germ cell mutagenicity**
Test Type: unscheduled DNA synthesis assay
Test system: mammalian cells
Metabolic activation: with and without metabolic activation
Result: negative

Test Type: Mutagenicity (mammal cell test): micronucleus.
Species: Mouse
Cell type: Bone marrow
Application Route: Oral
Method: OECD Test Guideline 474
Result: negative

Test Type: sister chromatid exchange assay
Species: Mouse
Cell type: Bone marrow
Application Route: Oral
Method: US-EPA
Result: negative

**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
Repeated dose toxicity - Rat - male - Oral - 28 d - NOAEL (No observed adverse effect level) - 9,200 mg/kg
Remarks: Subacute toxicity
(ECHA)

Repeated dose toxicity - Rat - female - Oral - 28 d - NOAEL (No observed adverse effect level) - 8,600 mg/kg
Remarks: Subacute toxicity
(ECHA)

Repeated dose toxicity - Rat - male - Oral - 92 d - NOAEL (No observed adverse effect level) - 6,800 mg/kg
Remarks: Subchronic toxicity
(ECHA)

Repeated dose toxicity - Rat - female - Oral - 92 d - NOAEL (No observed adverse effect level) - 7,200 mg/kg
Remarks: Subchronic toxicity
(ECHA)

RTECS: WG2100000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish
semi-static test LC50 - Oryzias latipes - 75 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates
static test EC50 - Daphnia magna (Water flea) - 70 mg/l - 48 h
(OECD Test Guideline 202)

Toxicity to algae
static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 77 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria
static test NOEC - activated sludge - > 100 mg/l - 3 h
12.2 Persistence and degradability

Biodegradability: aerobic - Exposure time 28 d
Result: 74.9 % - Readily biodegradable.

(ODC Test Guideline 301D)

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
No data available

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.

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.

SECTION 15: Regulatory information

SARA 302 Components

Aldrich - W392103
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.

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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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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