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

1.1 Product identifiers

Product name: \( p \)-Benzoquinone

Product Number: 12309
Brand: Sigma-Aldrich
Index-No.: 606-013-00-3
CAS-No.: 106-51-4

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)

Flammable solids (Category 1), H228
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Skin sensitization (Category 1), H317
Germ cell mutagenicity (Category 2), H341
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

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

2.2 GHS Label elements, including precautionary statements

Sigma-Aldrich - 12309
Pictogram

Signal word  Danger

Hazard statement(s)
H228  Flammable solid.
H301 + H331  Toxic if swallowed or if inhaled.
H314  Causes severe skin burns and eye damage.
H317  May cause an allergic skin reaction.
H335  May cause respiratory irritation.
H341  Suspected of causing genetic defects.
H410  Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)
P201  Obtain special instructions before use.
P202  Do not handle until all safety precautions have been read and understood.
P210  Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P240  Ground/bond container and receiving equipment.
P241  Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P260  Do not breathe dusts or mists.
P264  Wash skin thoroughly after handling.
P270  Do not eat, drink or smoke when using this product.
P271  Use only outdoors or in a well-ventilated area.
P272  Contaminated work clothing must not be allowed out of the workplace.
P273  Avoid release to the environment.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330  IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P301 + P330 + P331  IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353  IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310  IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310  IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P308 + P313  IF exposed or concerned: Get medical advice/ attention.
P333 + P313  If skin irritation or rash occurs: Get medical advice/ attention.
P363  Wash contaminated clothing before reuse.
P370 + P378  In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391  Collect spillage.
P403 + P233  Store in a well-ventilated place. Keep container tightly closed.
P405  Store locked up.
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: Quinone

Formula: \( \text{C}_6\text{H}_4\text{O}_2 \)

Molecular weight: 108.09 g/mol

CAS-No.: 106-51-4

EC-No.: 203-405-2

Index-No.: 606-013-00-3

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p )-benzoquinone</td>
<td>Flam. Sol. 1; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1; Muta. 2; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H228, H301, H331, H314, H318, H317, H341, H335, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1</td>
<td>&lt;= 100 %</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**

First aider needs to protect himself. Show this material safety data sheet to the doctor in attendance.

**If inhaled**

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

**In case of skin contact**

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

**In case of eye contact**

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

**If swallowed**

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.
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
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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
Remove container from danger zone and cool with water. 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 generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

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

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture.
Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-benzoquinone</td>
<td>106-51-4</td>
<td>TWA</td>
<td>0.1 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>0.1 ppm 0.4 mg/m3</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>0.1 ppm 0.4 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>0.1 ppm 0.4 mg/m3</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>0.1 ppm 0.4 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

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). Tightly fitting safety goggles

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 EN374 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 EN374 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**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when dusts 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. Risk of explosion.

---

**SECTION 9: Physical and chemical properties**

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

| a) Appearance | Form: powder |
| b) Odor | pungent |
| c) Odor Threshold | No data available |
| d) pH | 4 at 1 g/l at 20 °C (68 °F) - (External MSDS) |
| e) Melting point/freezing point | Melting point/range: 113 - 115 °C (235 - 239 °F) |
| f) Initial boiling point and boiling range | >= 160 °C >= 320 °F at 1,013 hPa - OECD Test Guideline 103 - Decomposes below the boiling point. |
| g) Flash point | 77 °C (171 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | The substance or mixture is a flammable solid with the category 1. - Test N.1: Test method for readily combustible solids |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | 0.133 hPa at 25 °C (77 °F) |
| l) Vapor density | No data available |
m) Relative density 1.33 at 20 °C (68 °F) - OECD Test Guideline 109
n) Water solubility 14.7 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water log Pow: 0.1 - 0.3 at 23 °C (73 °F) - Bioaccumulation is not expected.
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

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 bases
strong reducing agents
Risk of ignition or formation of inflammable gases or vapours with:
Sulfides
combustible substances
hydrides
Exothermic reaction with:
Oxidizing agents
alkalines
Strong acids

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
No data available

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 - 130 mg/kg
Remarks:
(RTECS)
Acute toxicity estimate Inhalation - 4 h - 0.51 mg/l
(Expert judgment)
Inhalation: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Dermal: No data available
No data available

Skin corrosion/irritation
Skin - in vitro test
Result: Corrosive after 3 minutes to 1 hour of exposure - 60 min
(OECD Test Guideline 431)

Serious eye damage/eye irritation
Causes serious eye damage.

Respiratory or skin sensitization
In Chemico Skin Sensitisation: Direct Peptide Reactivity Assay (DPRA) - In vitro study
Result: positive
(OECD Test Guideline 442C)

Germ cell mutagenicity
Suspected of causing genetic defects.
Ames test
S. typhimurium
Result: positive
Mutagenicity (micronucleus test)
Mouse - male and female
Result: positive
Remarks:
(ECHA)

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
Inhalation - May cause respiratory irritation. - Respiratory system

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available
11.2 Additional Information
RTECS: DK2625000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Damage to the eyes.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity
No data available

Toxicity to daphnia and other aquatic invertebrates
static test EC50 - Daphnia magna Straus (Water flea) - 0.13 mg/l - 48 h
(OECD Test Guideline 202)

Toxicity to algae
static test EC50 - Desmodesmus subspicatus (green algae) - 1.5 mg/l - 72 h
(OECD Test Guideline 201)

12.2 Persistence and degradability
Biodegradability
aerobic - Exposure time 28 d
Result: 56 % - Not rapidly biodegradable
(OECD Test Guideline 301A)

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 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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.
SECTION 14: Transport information

**DOT (US)**
- UN number: 2587
- Class: 6.1
- Proper shipping name: Benzoquinone
- Reportable Quantity (RQ): 10 lbs
- Poison Inhalation Hazard: No
- Packing group: II

**IMDG**
- UN number: 2587
- Class: 6.1
- Proper shipping name: BENZOQUINONE
- Marine pollutant: yes
- Packing group: II
- EMS-No: F-A, S-A

**IATA**
- UN number: 2587
- Class: 6.1
- Proper shipping name: Benzoquinone
- Packing group: II

SECTION 15: Regulatory information

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

**SARA 313 Components**
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-benzoquinone</td>
<td>106-51-4</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

**SARA 311/312 Hazards**
Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the
information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.8  Revision Date: 03/05/2021  Print Date: 07/11/2021