

• SAFETY DATA SHEET

Version 7.1
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 1,4-Benzoquinone (200 mg)
Product Number : 1056504
Brand : US Pharmacopeia
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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable solids : Category 1
Acute toxicity (Oral) : Category 3
Acute toxicity (Inhalation) : Category 3
Skin corrosion : Sub-category 1B

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Serious eye damage : Category 1
Skin sensitisation : Category 1
Germ cell mutagenicity : Category 2
Specific target organ toxicity - single exposure : Category 3 (Respiratory system)
Short-term (acute) aquatic hazard : Category 1
Long-term (chronic) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : 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 statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P260 Do not breathe dust.
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.

Response:

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.

P362 + P364 Take off contaminated clothing and wash it before reuse.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391 Collect spillage.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 106-51-4

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret



p-benzoquinone	106-51-4*	>= 80 - <= 100	TSC
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* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	: First aiders need to protect themselves. Show this 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.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
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Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Vapours 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.
Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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. Advice for emergency responders: For personal protection see section 8.
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- Environmental precautions : Do not let product enter drains.
Risk of explosion.
- 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.
- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
- Further information on storage conditions : Tightly closed.
Keep away from heat and sources of ignition.
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 4.1B, Flammable solid hazardous materials
- Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
p-benzoquinone	106-51-4	TWA	0.1 ppm 0.4 mg/m ³	OSHA Z-1
		SL	5 µg/100 cm ²	ACGIH
		TWA	0.1 ppm 0.4 mg/m ³	NIOSH REL
		TWA	0.1 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment



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.

Recommended Filter type: : Filter type P3

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.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : 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).

Eye 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 and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.



SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: powder
Color	: dark yellow
Odor	: pungent
Odor Threshold	: No data available
pH	: 4 (68 °F / 20 °C) Concentration: 1 g/l (External MSDS)
Melting point	: No data available
Boiling point/boiling range	: 320 °F / 160 °C (1,013 hPa) Decomposition: yes Method: OECD Test Guideline 103 Decomposes below the boiling point.
Flash point	: 171 °F / 77 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: The substance or mixture is a flammable solid with the category 1. Method: Test N.1: Test method for readily combustible solids
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: 0.133 hPa (77 °F / 25 °C)
Relative vapour density	: No data available
Relative density	: 1.33 (68 °F / 20 °C) Method: OECD Test Guideline 109
Density	: 1.32 g/cm ³ (68 °F / 20 °C)



Solubility(ies)	
Water solubility	: 14.7 g/l (68 °F / 20 °C) pH: 3.4 - 3.7 Method: OECD Test Guideline 105
Partition coefficient: n-octanol/water	: log Pow: 0.1 - 0.3 (73 °F / 23 °C) pH: 4.8 - 5.3 Method: OECD Test Guideline 107 Bioaccumulation is not expected.
Autoignition temperature	: 815 °F / 435 °C
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 108.1 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

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.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Strong bases strong reducing agents



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

Conditions to avoid : Strong heating.
Incompatible materials : Strong oxidizing agents
Hazardous decomposition : In the event of fire: see section 5 products

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 - dust/mist

(Expert judgement)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Dermal: No data available

Skin corrosion/irritation

Skin - in vitro assay

Result: Corrosive after 3 minutes to 1 hour of exposure - 60 min

(OECD Test Guideline 431)

Serious eye damage/eye irritation

Remarks: 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.

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 471

Result: positive

Test Type: In vivo micronucleus test

Species: Mouse



Application Route: Oral
Method: Mutagenicity (micronucleus test)
Result: positive
Remarks: (ECHA)

Carcinogenicity

IARC: No component 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 component 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

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

Ecotoxicity

Components:

p-benzoquinone:

Toxicity to fish : Remarks: No data available

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna Straus): 0.13 mg/l
End point: mortality
Exposure time: 48 h
Test Type: static test
Method: OECD Test Guideline 202



Toxicity to algae/aquatic plants : EC50 (Desmodesmus subspicatus (green algae)): 1.5 mg/l
Exposure time: 72 h
Test Type: static test
Method: OECD Test Guideline 201

Persistence and degradability

Components:

p-benzoquinone:

Biodegradability : aerobic
Inoculum: activated sludge, non-adapted
Result: Not rapidly biodegradable
Biodegradation: 56 %
Exposure time: 28 d
Method: OECD Test Guideline 301A

Bioaccumulative potential

Components:

p-benzoquinone:

Partition coefficient: n-octanol/water : log Pow: 0.1 - 0.3 (73 °F / 23 °C)
pH: 4.8 - 5.3
Method: OECD Test Guideline 107
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 2587
Proper shipping name : Benzoquinone
Class : 6.1
Packing group : II
Labels : Division 6.1 - Toxic substances
Packing instruction (cargo : 676
aircraft)
Packing instruction : 669
(passenger aircraft)

IMDG-Code

UN number : UN 2587
Proper shipping name : BENZOQUINONE

Class : 6.1
Packing group : II
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2587
Proper shipping name : Benzoquinone

Class : 6.1
Packing group : II
Labels : Division 6.1 - Toxic substances
ERG Code : 153
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.



SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
p-benzoquinone	106-51-4	10	10

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

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

p- 106-51-4 >= 90 - <= 100 %
benzoquinone

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

p-benzoquinone 106-51-4 >= 90 - <= 100 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

p-benzoquinone 106-51-4 >= 90 - <= 100 %

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

p-benzoquinone 106-51-4

Pennsylvania Right To Know

p-benzoquinone 106-51-4

Maine Chemicals of High Concern



Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
ACGIH / SL	:	Threshold Limit Value-Surface Limit (TLV-SL)
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); EC_x - Concentration associated with x% response; EHS - Extremely Hazardous Substance; EL_x - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErC_x - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC₅₀ - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC₅₀ - Lethal Concentration to 50 % of a test population; LD₅₀ - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed

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(Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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US / EN

