SAFETY DATA SHEET

1. Identification

Product identifier **Atovaquone**

Other means of identification

Catalog number 1044651

CAS number 95233-18-4

Chemical name 1,4-Naphthalenedione, 2-[4-(4-chlorophenyl)cyclohexyl]-3-hydroxy-, trans-

Recommended use Specified quality tests and assay use only.

Recommended restrictions Not for use as a drug. Not for administration to humans or animals.

Manufacturer/Importer/Supplier/Distributor information

Manufacturer

Company name U. S. Pharmacopeia

Address 12601 Twinbrook Parkway
Rockville
MD
20852-1790
United States

Telephone RS Technical Services 301-816-8129

Website www.usp.org

E-mail RSTECH@usp.org

Emergency phone number CHEMTREC within US & Canada 1-800-424-9300
CHEMTREC outside US & Canada +1 703-527-3887

2. Hazard(s) identification

Physical hazards Not classified.

Health hazards Not classified.

Environmental hazards Not classified.

OSHA defined hazards Not classified.

Label elements

Hazard symbol None.

Signal word None.

Hazard statement Not available.

Precautionary statement

Prevention Not available.

Response Not available.

Storage Not available.

Disposal Not available.

Hazard(s) not otherwise classified (HNOC) This product is supplied in a small quantity which does not constitute a combustible dust hazard. The physical properties of this material indicate that in large quantities accumulated dust may be hazardous.

Supplemental information Pharmacologically active material.

3. Composition/information on ingredients

Substance

Chemical name	Common name and synonyms	CAS number	%
Atovaquone		95233-18-4	100

4. First-aid measures

Inhalation If breathing is difficult, remove to fresh air and keep at rest in a position comfortable for breathing. Call a physician if symptoms develop or persist.

Skin contact Rinse skin with water/shower. Get medical attention if irritation develops and persists.

Eye contact Rinse with water. Get medical attention if irritation develops and persists.

Ingestion	Rinse mouth. If ingestion of a large amount does occur, call a poison control center immediately.
Most important symptoms/effects, acute and delayed	Pharmacologically active material. Occupational exposure may cause physiological effects.
Indication of immediate medical attention and special treatment needed	Treat symptomatically.
General information	Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

5. Fire-fighting measures

Suitable extinguishing media	Water. Foam. Dry chemical or CO2. Use fire-extinguishing media appropriate for surrounding materials.
Unsuitable extinguishing media	None known.
Specific hazards arising from the chemical	Explosion hazard: Avoid generating dust; fine dust dispersed in air in sufficient concentrations and in the presence of an ignition source is a potential dust explosion hazard.
Special protective equipment and precautions for firefighters	Wear suitable protective equipment.
Fire fighting equipment/instructions	Use water spray to cool unopened containers. As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.
Specific methods	Use standard firefighting procedures and consider the hazards of other involved materials.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Dust deposits should not be allowed to accumulate on surfaces, as these may form an explosive mixture if they are released into the atmosphere in sufficient concentration. Wear appropriate personal protective equipment. Avoid inhalation of dust from the spilled material. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	For waste disposal, see section 13 of the SDS. Avoid the generation of dusts during clean-up. Sweep up or vacuum up spillage and collect in suitable container for disposal. Clean surface thoroughly to remove residual contamination.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	As a general rule, when handling USP Reference Standards, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Avoid significant deposits of material, especially on horizontal surfaces, which may become airborne and form combustible dust clouds and may contribute to secondary explosions. Combustible dust clouds may be created where operations produce fine material (dust). Select and use containment devices and personal protective equipment based on a risk assessment of material potency and exposure potential.
Conditions for safe storage, including any incompatibilities	Store in tight container as defined in the USP-NF. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits

The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit. At this time, the other constituents have no known exposure limits.

Exposure limit values

Industrial Use

Material	Type	Value
Atovaquone (CAS 95233-18-4)	TWA	200 micrograms/m3

Biological limit values	No biological exposure limits noted for the ingredient(s).
Appropriate engineering controls	For laboratory operations, use local exhaust ventilation or a ventilated enclosure for high energy operations such as particle sizing. Control exposures to below the occupational exposure level (if available). Select and use containment devices and personal protective equipment based on a risk assessment of exposure potential. Cover all containers for solutions and slurries while being transferred.

Individual protection measures, such as personal protective equipment

Eye/face protection	Wear safety glasses with side shields, chemical splash goggles, or full face shield, if necessary. Base the choice of protection on the job activity and potential for contact with eyes or face. An emergency eye wash station should be available.
Skin protection	
Hand protection	Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.
Other	Train employees in proper gowning and degowning practices. Wear lab coat. Base the choice of skin protection on the job activity, potential for skin contact and solvents and reagents in use. Do not wear protective garments in common areas (e.g., cafeterias) or out-of-doors.
Respiratory protection	Respirators are generally not required for laboratory operations. Use a tight-fitting full-face respirator with HEPA filters for spill cleanup. Chose respiratory protection appropriate to the task and the level of existing engineering controls.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	Handling practices in this SDS are recommendations for laboratory use of reference standards. Procedures for any other uses or quantities should be determined after an appropriate assessment.

9. Physical and chemical properties

Appearance	Appearance descriptions are general information and not specific to any USP lot.
Physical state	Solid.
Form	Powder.
Color	Yellow.
Odor	Not available.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	420.8 - 426.2 °F (216 - 219 °C)
Initial boiling point and boiling range	Not available.
Flash point	Not available.
Evaporation rate	Not available.
Flammability (solid, gas)	Not available.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.
Explosive limit - upper (%)	Not available.
Vapor pressure	Not available.
Vapor density	Not available.
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Insoluble.
Solubility (other)	Methanol: Insoluble. Ethyl acetate: Slightly soluble. Alcohol: Slightly soluble. 1,3-butanediol: Slightly soluble. Polyethylene glycol 400: Sparingly soluble. Dimethyl sulfoxide: Sparingly soluble. Acetone: Sparingly soluble. Chloroform: Soluble. Tetrahydrofuran: Freely soluble. N-methyl-2-pyrrolidone: Freely soluble.
Partition coefficient (n-octanol/water)	5.31 at pH 7
Auto-ignition temperature	806 °F (430 °C)
Decomposition temperature	Not available.
Viscosity	Not available.

Other information

Chemical family	1,4-Hydroxynaphthoquinone.
Dust explosion properties	
Kst	368 bar.m/s
Minimum ignition energy (MIE) - dust cloud	3 - 4 mJ
Molecular formula	C22-H19-Cl-O3
Molecular weight	366.84 g/mol
pH in aqueous solution	6.3 - 6.4 10 % suspension
Specific gravity	0.17

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions. Cl-.

11. Toxicological information

Information on likely routes of exposure

Inhalation	Knowledge about health hazard is incomplete.
Skin contact	Knowledge about health hazard is incomplete.
Eye contact	Knowledge about health hazard is incomplete.
Ingestion	Knowledge about health hazard is incomplete.
Symptoms related to the physical, chemical, and toxicological characteristics	Fever. Skin rash. Gastrointestinal disturbances. Cough. Headache. Difficulty sleeping.

Information on toxicological effects

Acute toxicity

Product	Species	Test Results
Atovaquone (CAS 95233-18-4)		
Oral		
LD50	Mouse	> 2000 mg/kg
	Rat	> 2000 mg/kg

Skin corrosion/irritation Based on available data, the classification criteria are not met.

Serious eye damage/eye irritation Based on available data, the classification criteria are not met.

Local effects

Irritation test
Result: Negative.
Species: Rabbit
Organ: Eye
Irritation test, OECD 405
Result: Mild.
Species: Rabbit
Organ: Eye
Irritation test, OECD 405
Result: Negative.
Species: Rabbit
Organ: Skin

Respiratory or skin sensitization

Respiratory sensitization	Knowledge about health hazard is incomplete.
Skin sensitization	Knowledge about health hazard is incomplete.
Germ cell mutagenicity	Knowledge about mutagenicity is incomplete.

Mutagenicity

Ames test (Salmonella)
Result: Negative with and without activation.
Cultured human lymphocyte cytogenetic assay
Result: Negative.
In vivo mouse micronucleus assay
Result: Negative.
Mouse lymphoma mutagenesis assay
Result: Negative.

Carcinogenicity Not classifiable as to carcinogenicity to humans. Knowledge about carcinogenicity is incomplete.

Two-year carcinogenicity study
Result: Treatment-related increases in the incidence of hepatocellular adenoma and hepatocellular carcinoma at all doses tested.
Species: Mouse

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity Based on available data, the classification criteria are not met.

Reproductivity

Epidemiological study, 34 patients, 1st - 3rd trimesters
Result: No adverse developmental or reproductive effects.
Species: Human
Epidemiological study, Danish medical review, 242 patients
Result: No adverse developmental effects.
Species: Human
Reproductive study, 2 - 3 times the human dose
Result: No birth defects or adverse reproductive effects.
Species: Rat

Specific target organ toxicity - single exposure Knowledge about health hazard is incomplete.

Specific target organ toxicity - repeated exposure Knowledge about health hazard is incomplete.

Aspiration hazard Based on available data, the classification criteria are not met.

Further information Pharmacologically active material. Occupational exposure may cause physiological effects.

12. Ecological information

Ecotoxicity Very toxic to aquatic life with long lasting effects.

Product		Species	Test Results
Atovaquone (CAS 95233-18-4)			
Aquatic			
Acute			
Crustacea	EC50	Daphnia	0.0035 mg/l, 48 hours

Persistence and degradability No data is available on the degradability of this product.

Bioaccumulative potential

Octanol/water partition coefficient log Kow

5.31, @ pH 7

Mobility in soil No data available.

Other adverse effects No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions Dispose in accordance with all applicable regulations. Under RCRA, it is the responsibility of the user of the product to determine, at the time of disposal, whether the product meets RCRA criteria for hazardous waste.

Local disposal regulations Dispose in accordance with all applicable regulations.

Hazardous waste code The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information

DOT

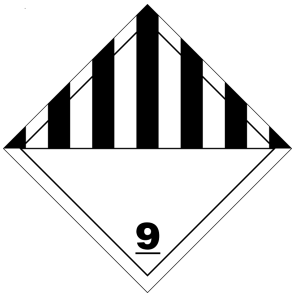
UN number UN3077
UN proper shipping name Environmentally hazardous substances, solid, n.o.s. (Atovaquone)
Transport hazard class(es)
Class 9
Subsidiary risk -
Packing group III
Packaging exceptions 155
Packaging non bulk 213
Packaging bulk 240

IATA

UN number UN3077
UN proper shipping name Environmentally hazardous substance, solid, n.o.s. (Atovaquone)
Transport hazard class(es)
Class 9
Subsidiary risk -
Packing group III
Other information
Passenger and cargo aircraft Allowed with restrictions.
Cargo aircraft only Allowed with restrictions.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

DOT; IATA



General information It is the shipper's responsibility to determine the correct transport classification at the time of shipment.

15. Regulatory information

US federal regulations This product is not known to be a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories Immediate Hazard - No
Delayed Hazard - No
Fire Hazard - Yes
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

SARA 313 (TRI reporting)

Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

US state regulations California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	No
Canada	Domestic Substances List (DSL)	No
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	No
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	No
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	No
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	No
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	No

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)
A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 05-29-2008

Revision date 02-06-2018

Version # 03

Further information Refer to NFPA 654, Standard for the Prevention of Fire and Dust Explosions from the Manufacturing, Processing, and Handling of Combustible Particulate Solids, for safe handling.

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