

SAFETY DATA SHEET

Creation Date 04-Oct-2019

Revision Date 20-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name Thymoquinone

Cat No. : AC305070000; AC305070010; AC305070050

CAS No 490-91-5
Synonyms 2-Isopropyl-5-methyl-1,4-benzoquinone

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Acute oral toxicity	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed
 May cause respiratory irritation
 Causes skin irritation
 Causes serious eye irritation



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
 Do not eat, drink or smoke when using this product
 Wear protective gloves/protective clothing/eye protection/face protection
 Avoid breathing dust/fume/gas/mist/vapors/spray
 Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
 Call a POISON CENTER or doctor if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
 If skin irritation occurs: Get medical advice/attention
 Take off contaminated clothing

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
 Rinse mouth

Storage

Store in a well-ventilated place. Keep container tightly closed
 Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	<=100

4. First-aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Chemical foam.
Unsuitable Extinguishing Media	No information available
Flash Point	103 °C / 217.4 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	0	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.
Environmental Precautions	Should not be released into the environment.
Methods for Containment and Clean Up	Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and Storage

Handling	Avoid ingestion and inhalation. Avoid dust formation. Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing.
Storage.	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible Materials. Acids. Oxidizing agent.

8. Exposure controls / personal protection

<u>Exposure Guidelines</u>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
Engineering Measures	Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.
<u>Personal Protective Equipment</u>	
Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

<u>Appearance</u>			
Physical State	Solid		
Color	Amber		
Odor	No information available		
Odor Threshold	No information available		
<u>Property</u>	<u>Values</u>	<u>Remarks</u>	<u>Method</u>
Melting Point/Range	43 - 44 °C / 109.4 - 111.2 °F		
Softening Point	No data available		
Boiling Point/Range	230 - 232 °C / 446 - 449.6 °F		
Flash Point	103 °C / 217.4 °F		
Flammability (liquid)	Not applicable		
Flammability (solid,gas)	No information available		Method - No information available
Explosion Limits	No data available		Solid
Autoignition Temperature	No data available		
Decomposition Temperature	No data available		
pH	No information available		
Viscosity	Not applicable		Solid
Water Solubility	Insoluble		
Solubility in other solvents	No information available		
Partition Coefficient (n-octanol/water)			
Vapor Pressure	No data available		
Density / Specific Gravity	No data available		
Bulk Density	No data available		
Vapor Density	Not applicable		Solid
Particle characteristics	No data available		
<u>Other Information</u>			
Molecular Formula	C10 H12 O2		
Molecular Weight	164.2		
Evaporation Rate	Not applicable - Solid		

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under recommended storage conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Acids, Oxidizing agent
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes. Irritating to eyes.
Skin	May cause irritation. Avoid contact with skin.

Toxicology data for the components

Toxicologically Synergistic Products	No information available
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	Not listed				

(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system.

(i) STOT-repeated exposure; No data available
 Target Organs No information available.

(j) aspiration hazard; Not applicable
 Solid

Other Adverse Effects

Symptoms / effects, both acute and delayed No information available.

Other Adverse Effects

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Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability Insoluble in water May persist based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	-	X	207-721-1	-	-		-	-	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
2,5-Cyclohexadiene-1,4-dione,	490-91-5	-	-	-

2-methyl-5-(1-methylethyl)-				
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Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-	490-91-5	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By	Product stewardship (Regulatory Affairs) Thermo Fisher Scientific email - begel.sdsdesk@thermofisher.com
Creation Date	04-Oct-2019
Revision Date	20-Dec-2025
Print Date	20-Dec-2025
Revision Summary	Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS