

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

Catalogue Number	CS-O-61943
Product Name	Thymoquinone-d6 (propan-2-yl-1,1,1,3,3,3-d6)
CAS No.	3057437-67-6
Category	Stable Isotopes
Synonyms	2-methyl-5-(propan-2-yl-1,1,1,3,3,3-d6)cyclohexa-2,5-diene-1,4-dione
Brand	Clearsynth Labs Ltd.
Identified uses	Laboratory Chemicals
Uses advised against	Not available
Company	Clearsynth Labs Ltd. Mumbai, India
Emergency Phone #	+91-22-245045900
REACH No.	Not available

SECTION 2: Hazards identification

Disclaimer: This is sample MSDS. Please email sales@clearsynth.com for more details.

2.1 Classification of the substance or mixture-Regulation (EC) No 1272/2008:

Not available

2.2 Label Elements

Signal Word: Not available

Not available

Hazard Statement(s)

Code	Statement
Not available	Not available

Precautionary Statement(s)

Code	Statement
Not available	Not available

SECTION 3: Composition / information on ingredients

3.1 Substance

Component : Thymoquinone-d6 (propan-2-yl-1,1,1,3,3,3-d6)
CAS Number : 3057437-67-6
Molecular Formula : C₁₀H₆D₆O₂
Molecular Weight : 170.24
Parent Chemical : Thymoquinone
Synonyms : 2-methyl-5-(propan-2-yl-1,1,1,3,3,3-d6)cyclohexa-2,5-diene-1,4-dione
Concentration : Not available

SECTION 4: First aid measures

SECTION 4: First-aid measures

4.1 Description of first aid measures

General advice: Seek medical attention if symptoms persist. Show this safety data sheet to the physician in attendance.

Inhalation: Move person to fresh air. If breathing is difficult, seek medical attention.

Skin contact: Wash with soap and water. Remove contaminated clothing and wash before reuse. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention if irritation persists.

Ingestion: Rinse mouth. Do not induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

Not available.

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. No data available.

SECTION 5: Firefighting measures

SECTION 5: Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media: Use extinguishing measures appropriate to surrounding fire (e.g., water spray, alcohol-resistant foam, dry chemical, carbon dioxide).

Unsuitable extinguishing media: Not available.

5.2 Special hazards arising from the substance or mixture

Specific hazards: No data available.

Hazardous combustion products: Not available.

5.3 Advice for firefighters

Wear self-contained breathing apparatus and full protective gear. Cool containers with water spray if exposed to fire.

Avoid inhalation of combustion products.

SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use appropriate personal protective equipment. Avoid breathing dust/vapors. Avoid contact with skin and eyes. Ensure adequate ventilation.

6.2 Environmental precautions

Avoid release to the environment. Prevent further leakage or spillage if safe to do so.

6.3 Methods and material for containment and cleaning up

Contain spill. Collect spilled material using methods that minimize dust generation. Place in a suitable, closed container for disposal. Clean contaminated area.

6.4 Reference to other sections

See Section 8 for personal protective equipment and Section 13 for disposal considerations.

SECTION-7: Handling and storage

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Handle in accordance with good industrial hygiene and safety practice. Avoid contact with skin and eyes. Avoid breathing dust/vapors. Use with adequate ventilation. Keep container tightly closed when not in use.

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated place. Protect from moisture. Keep in original container, tightly closed.

Incompatible materials: Not available.

7.3 Specific end use(s)

For laboratory/research use. Not for food, drug, or household use.

SECTION 8: Exposure controls / personal protection

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limits: Not available.

Biological limit values: Not available.

8.2 Exposure controls

Engineering controls: Provide adequate ventilation. Use local exhaust where dust/vapor may be generated.

Personal protective equipment (PPE):

- Eye/face protection: Safety glasses with side shields or chemical splash goggles.
- Skin protection: Protective gloves. Protective clothing as appropriate.
- Respiratory protection: If ventilation is inadequate, use appropriate respiratory protection.
- Hygiene measures: Wash hands after handling. Do not eat, drink, or smoke when using this product.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Test	Result
Appearance	No data available

Test	Result
IR spectrum	No data available
pH	No data available
Solubility	No data available

Property	Value
a) Physical State	No data available
b) Color	No data available
c) Odor	No data available
d) pH	No data available
e) Vapour Pressure	No data available
f) Viscosity	No data available
g) Initial Boiling Point and boiling range	No data available
h) Melting Point / Freezing Point	No data available
i) Auto Ignition Temperature	No data available
j) Flash Point	No data available
k) Explosion Limit, Lower	No data available
l) Explosion Limit, Upper	No data available
m) Decomposition Temperature	No data available
n) Loss on Drying	No data available
o) Relative Density	No data available
p) Solubility (in DMSO)	No data available
q) Oxidizing Properties	No data available

SECTION 10: Stability and reactivity

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available.

10.4 Conditions to avoid

Heat, open flame, and other ignition sources. Moisture (if applicable). Other conditions: Not available.

10.5 Incompatible materials

Not available.

10.6 Hazardous decomposition products

Not available.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

- Acute toxicity: No data available.
- Skin corrosion/irritation: No data available.
- Serious eye damage/eye irritation: No data available.
- Respiratory or skin sensitization: No data available.
- Germ cell mutagenicity: No data available.
- Carcinogenicity: No data available.
- Reproductive toxicity: No data available.
- STOT-single exposure: No data available.
- STOT-repeated exposure: No data available.
- Aspiration hazard: No data available.

Likely routes of exposure

- No data available.

Symptoms related to the physical, chemical and toxicological characteristics

- Not available.

SECTION 12: Ecological information

SECTION 12: Ecological information

12.1 Toxicity

Not available.

12.2 Persistence and degradability

Not available.

12.3 Bioaccumulative potential

Not available.

12.4 Mobility in soil

Not available.

12.5 Results of PBT and vPvB assessment

Not available.

12.6 Endocrine disrupting properties

Not available.

12.7 Other adverse effects

Not available.

SECTION 13: Disposal considerations

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Dispose of contents/container in accordance with local/regional/national/international regulations. Do not discharge to drains.

Waste classification: Not available.

Contaminated packaging: Dispose of as unused product or according to local regulations.

SECTION 14: Transport information

SECTION 14: Transport information

14.1 UN number

Not available.

14.2 UN proper shipping name

Not available.

14.3 Transport hazard class(es)

Not available.

14.4 Packing group

Not available.

14.5 Environmental hazards

Not available.

14.6 Special precautions for user

Not available.

14.7 Maritime transport in bulk according to IMO instruments

Not available.

SECTION 15: Regulatory information

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Not available.

15.2 Chemical safety assessment

Not available.

SECTION 16: Other information

SECTION 16: Other information

Product name: Thymoquinone-d6 (propan-2-yl-1,1,1,3,3,3-d6)

Catalog no.: CS-O-61943

CAS no.: 3057437-67-6

Category: Stable Isotopes

Molecular weight: 170.24

Synonyms: 2-methyl-5-(propan-2-yl-1,1,1,3,3,3-d6)cyclohexa-2,5-diene-1,4-dione

Parent chemical: Thymoquinone

Supplier: Clearsynth Labs Ltd., Mumbai, India

Emergency phone: +91-22-245045900

Revision date: Not available.

Disclaimer: The information provided is believed to be accurate based on available data; however, no warranty is expressed or implied. Users must determine suitability for their particular purpose and comply with applicable laws and regulations.

DISCLAIMER

This MSDS is system-generated. Please verify and confirm all data, statements, and values with the Support Team before use or distribution.