

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

Catalogue Number	CS-T-103796
Product Name	Thymoquinone-13C,d3
CAS No.	2714418-72-9
Category	Stable Isotopes
Synonyms	2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione-13C,d3; p-Mentha-3,6-diene-2,5-dione-13C,d3; 2-Isopropyl-5-methyl-1,4-benzoquinone-13C,d3; 2-Isopropyl-5-methyl-p-benzoquinone-13C,d3; 2-Isopropyl-5-methylbenzoquinone-13C,d3; 2-Methyl-5-isopropyl-1,4-benzoquinone-13C,d3; 2-Methyl-5-isopropyl-p-benzoquinone-13C,d3; 5-Isopropyl-2-methyl-1,4-benzoquinone-13C,d3; 5-Isopropyl-2-methyl-p-benzoquinone-13C,d3; NSC 2228-13C,d3; Thymoquinon-13C,d3; p-Cymene-2,5-dione-13C,d3;
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-13C,d3

CAS Number : 2714418-72-9

Molecular Formula : C¹³CH₁₀DO

Molecular Weight : 168.21

Parent Chemical : Thymoquinone

Synonyms : 2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione-13C,d3;

p-Mentha-3,6-diene-2,5-dione-13C,d3; 2-Isopropyl-5-methyl-1,4-benzoquinone-13C,d3;

2-Isopropyl-5-methyl-p-benzoquinone-13C,d3; 2-Isopropyl-5-methylbenzoquinone-13C,d3;

2-Methyl-5-isopropyl-1,4-benzoquinone-13C,d3; 2-Methyl-5-isopropyl-p-benzoquinone-13C,d3;

5-Isopropyl-2-methyl-1,4-benzoquinone-13C,d3; 5-Isopropyl-2-methyl-p-benzoquinone-13C,d3; NSC 2228-13C,d3;

Thymoquinon-13C,d3; p-Cymene-2,5-dione-13C,d3;

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 occur or persist. Show this SDS to the physician.

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

Skin contact: Wash with plenty of 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 local circumstances and the surrounding environment (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

Hazardous combustion products: Not available. Thermal decomposition may produce irritating and/or toxic fumes.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective gear. Cool containers with water spray if exposed to fire. Prevent fire-fighting water from entering drains or waterways.

SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

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

6.2 Environmental precautions

Avoid release to the environment. Prevent entry into drains, sewers, or waterways.

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, labeled container for disposal. Clean contaminated area with suitable cleaning method. Dispose of waste in accordance with local regulations.

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 formation of dust/aerosols. Avoid contact with skin, eyes, and clothing. Use with adequate ventilation.

7.2 Conditions for safe storage, including any incompatibilities

Store tightly closed in original container in a cool, dry, well-ventilated place. Protect from moisture. Incompatibilities: 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: No data available.

Biological limit values: Not available.

8.2 Exposure controls

Engineering controls: Use local exhaust ventilation or general ventilation to minimize exposure.

Personal protective equipment (PPE):

- Eye/face protection: Safety glasses with side shields or chemical splash goggles.
- Skin protection: Protective gloves (material not available). Wear protective clothing as appropriate.
- Respiratory protection: If ventilation is inadequate or exposure is possible, use a NIOSH/EN-approved respirator suitable for particulates/organic vapors as appropriate. Selection should be based on risk assessment.
- 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
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

Property	Value
p) Solubility (in DMSO)	No data available
q) Oxidizing Properties	No data available

SECTION 10: Stability and reactivity

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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, sparks, open flames, and other ignition sources (general precaution). Avoid dust generation. Other conditions: Not available.

10.5 Incompatible materials

Not available.

10.6 Hazardous decomposition products

Not available. May emit irritating and/or toxic fumes upon thermal decomposition.

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

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12.1 Toxicity

No data available.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

Not available.

12.6 Endocrine disrupting properties

No data available.

12.7 Other adverse effects

No data 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.

Recommended disposal: Incineration or disposal via a licensed chemical waste contractor, as appropriate.

Contaminated packaging: Dispose of as unused product.

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

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

Not available.

15.2 Chemical safety assessment

No data available.

SECTION 16: Other information

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CAS no.: 2714418-72-9

Supplier: Clearsynth Labs Ltd., Mumbai, India

Emergency phone: +91-22-245045900

Recommended use: Laboratory/research use.

Revision information: Not available.

Disclaimer: The information provided is believed to be accurate based on available data; however, it is provided without warranty. Users are responsible for determining suitability for their particular application and for compliance with applicable laws and regulations.

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