Safety Data Sheet

1,3,5-Trimethylbenzene-d_{12}

Section 1. Chemical product and company identifications

Product code: D-2911
Chemical formula: C_9D_{12}
CAS: 69441-16-3
CAS (unlabelled): 108-67-8
Synonyms: Mesitylene, *sym*-Trimethylbenzene

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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Pointe-Claire (Québec) H9R 1H1
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Website: www.cdnisotopes.com

In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid
Warning: Flammable liquid and vapour. Causes skin irritation.
Routes of entry: Inhalation, skin and eyes

GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

GHS Classification:
- Flammable liquids (Category 3)
- Acute toxicity, Oral (Category 5)
- Acute toxicity, Inhalation (Category 5)
- Skin corrosion/irritation (Category 2)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system

GHS Label elements:
- Pictograms:
- Signal word: Danger

Hazards statement:
- H226 Flammable liquid and vapour.
- H303 + H333 May be harmful if swallowed or if inhaled.
- H315 Causes skin irritation.
- H335 May cause respiratory irritation.

Precautionary statement:
- P210 Keep away from heat/hot surfaces/sparks/open flames/ignition sources. No smoking.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ eye protection/ face protection.
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
- P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER or doctor/ physician if you feel unwell.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
1,3,5-Trimethylbenzene-d_{12}	69441-16-3	> 98

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Section 4. First aid measures

Eye contact: Flush eyes with water as a precaution.
Skin contact: Wash off with soap and plenty of water. Consult a physician.
Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
Ingestion: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Section 5. Firefighting measures

Flammability of the product: Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.
Lower explosion limit: 0.9 Vol%
Upper explosion limit: 6.1 Vol%
Auto-ignition temperature: 550 °C (1,022 °F).
Flash point: 44 °C (111 °F) - closed cup.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.
Firefighting media and instructions: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
Special protective equipment for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Section 6. Accidental release measures

Personal precautions: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
Methods for cleaning up: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build-up of electrostatic charge.
Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources.

Section 8. Exposure Controls, Personal Protections

Engineering controls: Use mechanical exhaust or laboratory fumehood to avoid exposure.
Eyes: Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Respiratory: Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).
Hands: Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Skin/body: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Section 9. Physical and chemical properties (unlabelled)

Molecular weight: 120.19 g/mol
Physical status: Liquid
Color: Colourless
Odour: No data available
Density: 0.864 g/mL at 25 °C (77 °F)
Melting point: -45 °C (-49 °F) – lit.
Boiling point: 163 - 166 °C (325 - 331 °F) – lit.
Vapour pressure: 3.3 hPa (2.5 mmHg) at 25 °C (77 °F).
Vapour density: 4.2 (Air = 1)
Partition coefficient (octanol/water): log Pow: 3.42
Water solubility: 48.2 mg/L

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Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Strong oxidizing agents.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.
Reactivity conditions: Heat, flames and sparks.

Section 11. Toxicological information (unlabelled)

Toxicological data: Mesitylene

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Mesitylene	108-67-8	Oral - Rat - 5,000 mg/kg	Inhalation - Rat - 4 h - 24,000 mg/m^3

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** May be harmful if swallowed.

Potential chronic effects

- **Carcinogenic effects:** 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. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Mesitylene	12.52 mg/l LC50	Carassius auratus	96 h
	6 mg/l EC50	Daphnia magna	48 h

Effects on environment: An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Mobility: No data available.
Environmental precautions: No data available.
Persistence and degradability: No data available.
Bioaccumulative potential: No data available.

Section 13. Disposal considerations

Waste disposal: Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: 1,3,5-Trimethylbenzene
UN number: UN2325
Class: 3
Packaging group: III

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 2
Flammable: 2
Reactivity: 0
Specials conditions: None

Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous

U.S. Federal regulations:

TSCA 8(b) inventory: Mesitylene
SARA 302/304/311/312 extremely hazardous substances: Not Listed
SARA 302/304 emergency planning and notification: Not Listed
SARA 302/304/311/312 hazardous chemicals: Not Listed
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Not Listed
CWA (Clean Water Act) 307: Not Listed
CWA (Clean Water Act) 311: Not Listed
CAA (Clean Air Act) 112 accidental release prevention: Not Listed
CAA (Clean Air Act) 112 regulated flammable substances: Not Listed
CAA (Clean Air Act) 112 regulated toxic substances: Not Listed

State regulations:

DEA List I Chemicals (Precursor Chemicals): Not Listed
DEA List II Chemicals (Essential Chemicals): Not Listed
Substances in Massachusetts: Not Listed
Dangerous substances in New Jersey: Not Listed
New York – Dangerous substances with acute effects: Not Listed
Dangerous substances in Pennsylvania – right to know: Not Listed

WHMIS (Canada):

B3 – Combustible liquid

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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Elaborated by: **Toxyscan Inc., 1-866-780-0599**
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