

Toluene-2,3,4,5,6-d₅

Section 1. Chemical product and company identifications

Product code: D-0351

Chemical formula: C₇H₃D₅

CAS: 1603-99-2

CAS (unlabelled): 108-88-3

Synonyms: Methylbenzene, Toluol

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid

Warning: Highly flammable liquid and vapour. Causes skin irritation. Causes serious eye irritation.

Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:

- Flammable liquids (Category 2)
- Acute toxicity, Oral (Category 4)
- Skin irritation (Category 2)
- Eye irritation (Category 2A)
- Reproductive toxicity (Category 2)
- Specific target organ toxicity - single exposure (Category 3), Central nervous system
- Specific target organ toxicity - repeated exposure (Category 2)
- Aspiration hazard (Category 1)

GHS Label elements:

- Pictograms:   
- Signal word: Danger

Hazards statement:

- H225 Highly flammable liquid and vapour.
- H302 Harmful if swallowed.
- H304 May be fatal if swallowed and enters airways.
- H315 Causes skin irritation.
- H319 Causes serious eye irritation.
- H336 May cause drowsiness or dizziness.
- H361 Suspected of damaging fertility or the unborn child.
- H373 May cause damage to organs through prolonged or repeated exposure.

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/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P302 + P350 IF ON SKIN: Wash with plenty of soap and water.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P316 Get emergency medical help immediately.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
Toluene-2,3,4,5,6-d ₅	1603-99-2	> 98

Section 4. First aid measures

Eye contact: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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: 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: 1.1 Vol%

Upper explosion limit: 7.1 Vol%

Auto-ignition temperature: 535 °C (995 °F)

Flash point: 4 °C (39 °F)

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.

Environmental precautions: Do not let product enter drains. Discharge into the environment must be avoided.

Methods for cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking.

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: Safety glasses with side-shields conforming to 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: 92.14 g/mol

Physical status: Liquid

Color: Clear

Odour: Aromatic

Density: 0.865 g/ml

Melting point: -95 °C (-139 °F)

Boiling point: 110 - 111 °C (230 - 232 °F)

Vapour pressure: 29 hPa (22 mmHg) at 20 °C (68 °F)

Vapour density: 3.1 (Air = 1)

Partition coefficient (octanol/water): log Pow: 2.73

Water solubility: 0.53 g/L

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: Toluene

Information on ingredients:

Name	CAS	LD₅₀	LC₅₀
Toluene	108-88-3	Oral - Rat - 636 mg/kg	Inhalation - Rat - 4 h - 49,000 mg/m ³

Potential acute effects

- **Eyes:** Causes serious eye irritation.
- **Skin:** May be harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
- **Ingestion:** Harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

Potential chronic effects

- **Carcinogenic effects:** This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification. IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Toluene). 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:** Suspected of damaging the unborn child. Suspected human reproductive toxicant.
- **Medical conditions aggravated by overexposure:** May cause damage to organs through prolonged or repeated exposure.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Toluene	25 mg/l LC50	Oryzias latipes	96 h
	4.1 mg/l EC50	Daphnia magna	48 h
	29 mg/l EC50	Selenastrum capricornutum	72 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: Aerobic. Result: 86 % - Readily biodegradable.

Bioaccumulative potential: Leuciscus idus - 3 d - 0.05 mg/l. Bioconcentration factor (BCF): 90.

Section 13. Disposal considerations

Waste disposal: Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Toluene

UN number: UN1294

Class: 3

Packaging group: II

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 2
Flammable: 3
Reactivity: 0
Special conditions: None

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

U.S. Federal regulations:

TSCA 8(b) inventory: Toluene

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: 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: Listed

Dangerous substances in New Jersey: Listed

New York – Dangerous substances with acute effects: Not Listed

Dangerous substances in Pennsylvania – right to know: Listed

WHMIS (Canada):



B2 - Flammable liquid



D2A - Very toxic material causing other toxic effects
D2B - Toxic material causing other toxic effects

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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