Safety Data Sheet

Ethylbenzene-2,3,4,5,6-d_5

Section 1. Chemical product and company identifications

Product code: D-1903
Chemical formula: $C_8H_5D_5$
CAS: 20302-26-5
CAS (unlabelled): 100-41-4
Synonyms: Phenylethane

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. Harmful if inhaled.
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, Inhalation (Category 4)
- 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.
- H304 May be fatal if swallowed and enters airways.
- H332 Harmful if inhaled.
- 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.
- P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- 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.
- P312 Call a POISON CENTER or doctor/ physician if you feel unwell.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
Ethylbenzene-2,3,4,5,6-d_5	20302-26-5	> 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: 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 Vol%
Upper explosion limit: 6.7 Vol%
Auto-ignition temperature: 432 °C (810 °F)
Flash point: 15 °C (59 °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: 106.17 g/mol
Physical status: Liquid
Color: Colorless
Odour: Aromatic
Density: 0.867 g/mL
Melting point: -95 °C (-139 °F)
Boiling point: 136 °C (277 °F)
Vapour pressure: 13.3 hPa (10 mmHg) at 20 °C (68 °F)
Vapour density: 3.7 (Air = 1)
Partition coefficient (octanol/water): log Pow: 3.15
Water solubility: 0.2 g/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: Ethylbenzene

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Ethylbenzene	100-41-4	Oral - Rat - 3,500 mg/kg	No data available

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. Aspiration hazard if swallowed - can enter lungs and cause damage.

Potential chronic effects

- **Carcinogenic effects:** IARC: 2B - Group 2B: Possibly carcinogenic to humans (Ethylbenzene).
- **Mutagenic effects:** Genotoxicity in vitro - Hamster - ovary - with and without metabolic activation – negative. Genotoxicity in vivo - Mouse - male and female – negative.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Ethylbenzene	5.1 mg/l LC50	Menidia menidia	96 h
	1.8 - 2.4 mg/l EC50	Daphnia magna	48 h
	4.9 mg/l EC50	Skeletonema costatum	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: Readily biodegradable
Bioaccumulative potential: No data available.

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: Ethylbenzene
UN number: UN1175
Class: 3
Packaging group: II

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 1
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: Ethylbenzene
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: Listed
CWA (Clean Water Act) 311: Listed
CAA (Clean Air Act) 112 accidental release prevention: Listed
CAA (Clean Air Act) 112 regulated flammable substances: Listed
CAA (Clean Air Act) 112 regulated toxic substances: 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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