Safety Data Sheet

2-Phenylpropane-1,1,1,2,3,3,3-d_7

Section 1. Chemical product and company identifications

Product code: D-0681
Chemical formula: $C_9H_5D_7$
CAS: 20201-28-9
CAS (unlabelled): 98-82-8
Synonyms: Cumene, Isopropylbenzene

Supplier / Manufacturer:

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In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

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

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

GHS Classification:
- Flammable liquids (Category 3)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system
- Aspiration hazard (Category 1)

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

Hazards statement:
- H226 Flammable liquid and vapour.
- H304 May be fatal if swallowed and enters airways.
- 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.
- P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
2-Phenylpropane-1,1,1,2,3,3,3-d_7	20201-28-9	> 98

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.

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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: 6.5 Vol%
Auto-ignition temperature: 425 °C (797 °F)
Flash point: 31 °C (88 °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: Colorless
Odour: No data available
Density: 0.864 g/mL
Melting point: -96 °C (-141 °F) – lit.
Boiling point: 152 - 154 °C (306 - 309 °F) - lit.
Vapour pressure: 10.7 hPa (8 mmHg) at 20 °C (68 °F)
Vapour density: No data available
Partition coefficient (octanol/water): log Pow: 3.66
Water solubility: 61 mg/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Strong oxidizing agent.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.
Reactivity conditions: Heat, flames and sparks. Vapours may form explosive mixture with air.

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Section 11. Toxicological information (unlabelled)

Toxicological data: Isopropylbenzene

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Isopropylbenzene	98-82-8	Oral - Rat - 1,400 mg/kg	No data available

Potential acute effects

- **Eyes:** Causes eye irritation.
- **Skin:** May be harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. Causes 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 (Cumene). 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:** Genotoxicity in vitro - in vitro assay - S. typhimurium - with and without metabolic activation – negative. Genotoxicity in vivo - Mouse - male and female - inhalation (gas) – negative.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Isopropylbenzene	4.8 mg/l LC50	Oncorhynchus mykiss	96 h
	2.14 mg/l EC50	Daphnia	48 h
	2.60 mg/l EC50	Pseudokirchneriella subcapitata	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: According to the results of tests of biodegradability this product is not readily biodegradable.
Bioaccumulative potential: No data available.

Section 13. Disposal considerations

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

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Isopropylbenzene
UN number: UN1918
Class: 3
Packaging group: III

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 2
Flammable: 3
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: Isopropylbenzene
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):

B2 - Flammable liquid

D2A - Very 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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