Safety Data Sheet

(±)-Ibuprofen-d_3 (α-methyl-d_3)

Section 1. Chemical product and company identifications

Product code: D-6119
Chemical formula: $C_{13}H_{15}D_3O_2$
CAS: 121662-14-4
CAS (unlabelled): 15687-27-1
Synonyms: α-Methyl-4-(isobutyl)phenylacetic Acid, (±)-2-(4-Isobutylphenyl)propanoic Acid

Supplier / Manufacturer:

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In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Solid
Warning: Harmful if swallowed. Causes serious eye irritation.
Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:
- Acute toxicity, Oral (Category 4)
- Eye irritation (Category 2A)
- Specific target organ toxicity - single exposure (Category 3)

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

Hazards statement:
- H302 Harmful if swallowed.
- H319 Causes serious eye irritation.
- H335 May cause respiratory irritation.

Precautionary statement:
- 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.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P312 Call a POISON CENTER or doctor/ physician if you feel unwell.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
(±)-Ibuprofen-d_3	121662-14-4	> 98

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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: Not flammable or combustible.
Lower explosion limit: No data available
Upper explosion limit: No data available
Auto-ignition temperature: No data available
Flash point: No data available
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 dust formation. Ensure adequate ventilation. Avoid breathing dust.
Environmental precautions: Do not let product enter drains.
Methods for cleaning up: Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation.
Storage: Store at room temperature. Adequate ventilation.

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: 206.28 g/mol
Physical status: Solid
Color: White to off-white
Odour: No data available
Density: No data available
Melting point: 77 - 78 °C (171 - 172 °F)
Boiling point: No data available
Vapour pressure: No data available
Vapour density: No data available
Partition coefficient (octanol/water): log Pow: 3.97
Water solubility: 21 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: No data available.

Section 11. Toxicological information (unlabelled)

Toxicological data: Ibuprofen

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
Ibuprofen	15687-27-1	Oral - Rat - 636 mg/kg	No data available

Potential acute effects

- **Eyes:** Causes serious eye irritation.
- **Skin:** Harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** 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:** Possible risk of congenital malformation in the fetus.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
Ibuprofen	No data available		

Effects on environment: No data available
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.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Not dangerous goods
UN number: None
Class: None
Packaging group: None

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 2
Flammable: 0
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: Ibuprofen
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: 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):

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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