

Ibandronate sodium monohydrate SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Ibandronate sodium monohydrate

* Catalog Number: S3148

* CAS Number: 138926-19-9

* IUPAC Name: Phosphonic acid, P,P'-[1-hydroxy-3-(methylpentylamino)propylidene]bis-, sodium salt, hydrate (1:1:1)

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals

* TollFree: +1 877 796-6397

* Tel: +1 832 582-8158

* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity (oral): Category 4. H302

Acute toxicity (dermal): Category 4. H312

Skin corrosion: Category 1. H314

Skin irritation: Category 2. H315

Serious eye damage: Category 1. H318

Serious eye irritation: Category 2. H319

Acute toxicity (inhalation): Category 4. H332

Specific target organ toxicity (single exposure): Category 3. H335

Carcinogenicity: Category 2. H351

Not classified. H360D

Reproductive toxicity: Category 2. H361

Reproductive toxicity: Category 1B. H362

Specific target organ toxicity (single exposure): Category 2. H371

Specific target organ toxicity (repeated exposure): Category 2. H373

Acute aquatic toxicity: Category 1. H400

Chronic aquatic toxicity: Category 1. H410

Chronic aquatic toxicity: Category 2. H411

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H302: Harmful if swallowed
H312: Harmful in contact with skin
H314: Causes severe skin burns and eye damage
H315: Causes skin irritation
H318: Causes serious eye damage
H319: Causes serious eye irritation
H332: Harmful if inhaled
H335: May cause respiratory irritation
H351: Suspected of causing cancer
H360D: May damage the unborn child
H361: Suspected of damaging fertility or the unborn child
H362: May cause harm to breast-fed children
H371: May cause damage to organs
H373: May causes damage to organs through prolonged or repeated exposure
H400: Very toxic to aquatic life
H410: Very toxic to aquatic life with long lasting effects
H411: Toxic to aquatic life with long lasting effects

Precautionary statement(s)

None.

Prevention

P203: Obtain, read and follow all safety instructions before use.
P260: Do not breathe dust/fume/gas/mist/vapors/spray.
P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
P263: Avoid contact during pregnancy/while nursing.
P264: Wash hands thoroughly after handling.
P264+P265: Wash hands thoroughly after handling. Do not touch eyes.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P273: Avoid release to the environment.
P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Response	P301+P317: IF SWALLOWED: Get medical help. P301+P330: IF SWALLOWED: Rinse mouth. P302+P352: IF ON SKIN: wash with plenty of water. P302+P361: IF ON SKIN: Take off immediately all contaminated clothing. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P305+P354: IF IN EYES: Immediately rinse with water for several minutes. P308+P316: IF exposed or concerned: Get emergency medical help immediately. P316: Get emergency medical help immediately. P317: Get emergency medical help. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P331: Do NOT induce vomiting. P332+P317: If skin irritation occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P354: Immediately rinse with water for several minutes. P362+P364: Take off contaminated clothing and wash it before reuse. P363: Wash contaminated clothing before reuse. P391: Collect spillage.
Storage	P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Ibandronate sodium monohydrate

CAS Number: 138926-19-9

PubChem CID: 23663991

Molecular formula: C₉H₂₄NNaO₈P₂

Molecular weight: 359.23 g/mol

IUPAC name: sodium;hydroxy-[1-hydroxy-3-[methyl(pentyl)amino]-1-phosphonopropyl]phosphinate;hydrate

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Combustible. Heating may produce toxic fumes.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Sweep up or absorb with inert material (e.g., sand, vermiculite).

Place in sealed, labeled container for disposal.

Wash spill area with water.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Handle in accordance with good industrial hygiene and safety practices.

Wear appropriate PPE (see Section 8). Avoid contact with skin, eyes, and clothing.

Wash hands thoroughly after handling. Do not eat, drink, or smoke in work area.

Avoid dust formation. Use only in a chemical fume hood or well-ventilated area.

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles and face shield.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Solid powder (typical for research compounds)

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: No data available

f) Initial boiling point and boiling range: No data available

- g) Flash point: No data available
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: Soluble in DMSO; slightly soluble in water
- o) Partition coefficient: n-octanol/water: Log P: No data available
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 142 Å²

Complexity: 377

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Phosphorus oxides (P₂O₅).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

Causes severe skin burns and eye damage (H314).

Serious eye damage/eye irritation:

Causes serious eye damage (H318).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

Suspected of causing cancer (H351).

Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

Specific target organ toxicity (single exposure):

H371, H373

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

No indication of carcinogenicity to humans (not listed by IARC).

Exposure routes:

Poorly absorbed (mean bioavailability following a 2.5 mg oral dose is about 0.6% compared to intravenous dosing).
Absorption is impaired by any kind of food or drink other than plain water.

Signs and symptoms of exposure:

LD₅₀ = 811 mg/kg (rat, oral), side effects include bronchitis, pneumonia and urinary tract infections.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No ecotoxicity data available.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

This substance is classified as hazardous to the aquatic environment.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: Yes (classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Not available in public databases.

EU ECHA / REACH: Not available in public databases.

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute (short-term) health hazard
Chronic (long-term) health hazard
Environmental hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.