

3-Phospho-D-glyceric Acid Barium Salt Dihydrate

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Linear Formula	C ₃ H ₅ BAO ₇ P ₂ H ₂ O
Pubchem CID	91658989
MDL Number	MFCD00067190
EC No.	245-012-9
IUPAC Name	barium(2+); [(2R)-2-carboxy-2-hydroxyethyl] phosphate; dihydrate
SMILES	C(C(C(=O)O)OP(=O)([O-])[O-].O.O.[Ba+2]
Inchi Identifier	InChI=1S/C3H7O7P.Ba.2H2O/c4-2(3(5)6)1-10-11(7,8)9;;;h2,4H,1H2,(H,5,6)(H2,7,8,9);;2*1H2/q;+2;::p-2/t2-;;/m1.../s1
Inchi Key	IRPUBTOBTBTBNU-QYUNTSNKSA-L

Signal Word	Danger
Hazard Statements	H301+H331
Hazard Codes	T
Risk Codes	N/A
Safety Statements	N/A
Transport Information	UN1564 6.1/PG III

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SAFETY DATA SHEET

Date Accessed: 05/23/2024

Date Revised: 01/15/2022

SECTION 1. IDENTIFICATION

Product Identifiers: All applicable American Elements product codes for CAS #22457-55-2

Relevant identified uses of the substance:
Scientific research and development

Supplier details:
American Elements
10884 Weyburn Ave.
Los Angeles, CA 90024
Tel: +1 310-208-0551
Fax: +1 310-208-0351

Emergency telephone number:
Domestic, North America +1 800-424-9300
International +1 703-527-3887

SECTION 2. HAZARDS IDENTIFICATION

Statement of Hazard: Irritant, Respiratory irritant, Toxic

Acute Health Hazard: Irritant to eyes, skin, mucous membranes and respiratory system.

May be toxic by ingestion, skin absorption and inhalation.

Chronic Health Hazard: Not Available

HMIS Rating:

NFPA Rating:

To the best of our knowledge, the toxicological properties of this chemical have not been thoroughly investigated. Use appropriate procedures and precautions to prevent or minimize exposure.

Pictogram:



Signal Word: Warning

Hazard Statement(s): H301 Toxic if swallowed.

H311 Toxic in contact with skin.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H331 Toxic if inhaled.

H335 May cause respiratory irritation.

Precautionary Statement(s): P261 Avoid breathing dust/fume/gas/mist/vapors/spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink, or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position 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.

P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Chemical Name: D-3-Phosphoglyceric acid barium salt dihydrate 98%

Synonyms: Barium 3-phospho-D-glycerate

CAS Number: 22457-55-2

MDL Number: MFCD00067190

EINECS Number: 245-012-9

Beilstein Registry Number: Not Available

Molecular Formula: $C_3H_5BaO_7P \cdot 2H_2O$

Molecular Weight: 357.40

Content: As specified in product name.

SECTION 4. FIRST AID MEASURES

Eye Contact:

Skin Contact:

Ingestion:

Inhalation:

Flush eyes with large amounts of water for fifteen minutes. Separate eyelids with fingers. If irritation persists, seek medical attention.

Wash skin with soap and water. If irritation persists, seek medical attention.

Do not induce vomiting. Seek medical attention.

Move to a fresh air environment. Contact a physician if breathing becomes difficult.

SECTION 5. FIREFIGHTING MEASURES

Flash Point (°C):

Explosion Limits:

Not Available

Not Available

Auto Ignition

Temperature (°C):

Not Available

Carbon dioxide, dry chemical powder, alcohol-resistant foam, or water spray

Extinguishing Media:

Protective Equipment:

Specific Hazards:

Wear self-contained respirator and fully protective impervious suit.

May emit hazardous fumes under fire conditions.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal Protection: Wear a self-contained breathing apparatus, rubber boots and gloves, and disposable coveralls. Dispose of coveralls after use. Remove from ignition sources if safe to do so. Follow emergency response plan and contact proper authorities if needed.

Keep unprotected persons away.

Environmental Protection: Keep spills out of sewers and bodies of water. Dike and contain the spill with inert material. Absorb on sand, vermiculite or diatomite.

Transfer material to a container for disposal or recovery. Ventilate area and wash spill site after material pickup is complete.

SECTION 7. HANDLING AND STORAGE

Handling and Storage: Avoid breathing dust, vapor, mist or gas. Avoid contact with skin and eyes. Avoid prolonged or repeated exposure. Use only in a chemical fume hood. Open and handle container with care. Keep ignition sources away.

Store in a tightly closed container in a dry, well-ventilated place.

Hygroscopic, store away from water.

Sensitivities:

Storage Temperature (°C):

Hygroscopic, Light

-20

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering Controls: Use product in a well ventilated area or under a fume hood. Use proper lab equipment while handling this product. Keep away from incompatible materials for possible risk of hazardous reaction.

Eye Protection: Wear appropriate protective eyeglass or chemical safety goggles. Make sure that there is an eyewash station in your vicinity.

Skin Protection: Wear impervious gloves and protective clothing.

Respiratory Protection: Use a NIOSH approved respirator when exposure limits are exceeded or if irritation or other symptoms are experienced.

Exposure Limits: Country Source Type Value

USA

USA

USA

ACGIH

OSHA

OSHA

TWA

STEL

PEL

Not Available

Not Available

Not Available

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance:

SECTION 9: PHYSICAL and CHEMICAL PROPERTIES

Odor:

Odor Threshold:

Flash Point (°C):

Auto Ignition

Temperature (°C):

UEL % by Volume:

LEL % by Volume:

Melting Point (°C):

Boiling Point (°C):

Not Available

White powder

Not Available

Not Available

Not Available

Not Available

Not Available

Not Available

Not Available

Evaporation Rate:

pH Value:

Density (g/cm³):

Refractive Index (n²⁰D):

Viscosity:

Solubility in Water:

Solubility in Other:

Vapor Pressure (mmHg):

Vapor Density (Air=1):

Not Available

Not Available

Not Available

Not Available
Not Available
Not Available
Soluble in hydrochloric acid
Not Available
Not Available

SECTION 10. STABILITY AND REACTIVITY

Stability: Stable under normal temperatures and pressures.

Incompatibility: Strong oxidizing agents

Reactivity: Product may react with incompatible materials to release other hazardous substances.

Conditions to Avoid: Heat, flame, sparks, other ignition sources.

Hazardous

Decomposition Products:

Barium oxides, Carbon oxides, Phosphorus oxides

SECTION 11. TOXICOLOGICAL INFORMATION

RTECS Reference:

Target Organs: Not Available

Not Available

Toxicity Data: Not Available

National Toxicology Program (NTP) listed:

Not Available

Carcinogenicity:

International Agency for Research on Cancer (IARC) listed:

Not Available

Potential Symptoms: Not Available

SECTION 12. ECOLOGICAL INFORMATION

Toxicity: Not Available

SECTION 13. DISPOSAL CONSIDERATIONS

Contact a licensed professional waste disposal service. Dispose in a manner consistent with federal, state and local environmental regulations.

SECTION 14. TRANSPORT INFORMATION

DOT Shipping Name:
DOT UN Number:
DOT Hazard Class:
DOT Packing Group:
Barium Compound, N.O.S.
UN1564
Class 6.1
PGIII
IMDG Shipping Name: Barium Compound, N.O.S.
IMDG UN Number: UN1564
IMDG Hazard Class: Class 6.1
IMDG Packing Group: PGIII
Marine Pollutant: No
IATA: Barium Compound, N.O.S.
IATA UN Number: UN1564
IATA Hazard Class: Class 6.1
IATA Packing Group: PGIII

SECTION 15. REGULATORY INFORMATION

United States
Toxic Substance Control Act (TSCA) listed: No
Superfund Amendments and Reauthorization Act
(SARA 302) listed: No
Superfund Amendments and Reauthorization Act
(SARA 311/312) listed: No
Superfund Amendments and Reauthorization Act
(SARA 313) listed: No
European Union
European Inventory of Existing Chemical Substances
(EINECS): 245-012-9
Canada
Canadian Domestic Substances List (DSL) listed: No
Canadian Non-Domestic Substances List (NDSL)
listed: No

16. OTHER INFORMATION

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH). The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. American Elements shall not be held

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