1. Product and Company Identification

PRODUCT IDENTIFIER: Diborane (B2H6)

PRODUCT USE: Dopant for semiconductors, hydroboration and reduction reactions

CHEMICAL FAMILY: Boron hydrides

MANUFACTURED BY: Callery Chemical Company
Division of Mine Safety Appliances Company
PO Box 429; Pittsburgh, PA 15230
Callery Customer Service: 1-412-967-4141
Callery 24-Hour Telephone: 1-412-967-4100
Transportation Emergency: 1-800-424-9300 in USA or 1-703-527-3887 outside USA

2. Composition/Information on Ingredients

Diborane (CASRN: 19287-45-7)   wt%   Synonym(s)
> 99                      B2H6


Indications of danger (Annex II): Extremely flammable, Toxic, and Irritant
Nature of special risk attributed to dangerous substances (Annex III): R12, R23, R36/38
Safety advice concerning dangerous chemical substances (Annex IV): S24/25, S35, S36, S45, S46

3. Hazards Identification

EMERGENCY OVERVIEW: Colorless gas at room temperature with irritating, sickly sweet, unpleasant, distinctive odor. Liquid diborane is colorless. May be fatal if inhaled. Flammable gas. May cause flash fire or explosion. Causes respiratory tract irritation. May cause lung, kidney, and central nervous system effects. Reacts rapidly with water and alcohols generating flammable hydrogen gas. Can ignite on contact with air. May form explosive mixtures with air.

PHYSICAL HAZARDS: Flammable gas. May cause flash fire or explosion. Can ignite on contact with air. May form explosive mixtures with air.

POTENTIAL HEALTH EFFECTS: May be fatal if inhaled. Causes respiratory tract irritation. May cause lung, kidney, and central nervous system damage
- Primary Routes of Entry: Eye and skin contact, inhalation
- Target Organs: Eyes, skin, respiratory tract, central nervous system, kidneys, liver
- Medical Conditions Generally Recognized as Aggravated by Exposure: Persons with preexisting skin, respiratory, liver, kidney, and central nervous system conditions may be more susceptible to the effects of this product.
- Carcinogenicity: Diborane is not listed in the National Toxicology Program (NTP) Annual Report on Carcinogens, not found to be a potential carcinogen in the International Agency for Research on Cancer (IARC) Monographs, and not listed as an OSHA carcinogen.

POTENTIAL ENVIRONMENTAL EFFECTS: No environmental toxicity data for the product. See Section 12 for additional information.
4. First Aid Measures

INHALATION POISON! CAUSES THERMAL BURNS!
SEND TO A PHYSICIAN IMMEDIATELY IN ALL CASES.

Note: Immediately flushing with plenty of water is the appropriate eye and skin emergency first aid treatment for this water-reactive chemical. For the eye, it is extremely important that flushing with water (with the eyelids held open) begins within the first minute after diborane has entered the eye and continues for the full 20 minutes.

Eyes: Immediately flush eyes with plenty of water for at least 20 minutes while holding eyelids open.

Skin: Immediately flush skin with plenty of cool water for at least 20 minutes while removing contaminated clothing and shoes. Dispose of contaminated clothing and shoes in compliance with all local, state, and federal laws and regulations.

Ingestion: For any accidental contamination of the mouth, gargle with water and rinse mouth thoroughly. Then give two glasses of water, followed by demulcent such as milk, olive oil, or margarine in small amounts up to 2 or 3 ounces. Encourage, but do not force, vomiting. Never give anything by mouth to an unconscious person.

Inhalation: Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

5. Fire Fighting Measures

Flashpoint (closed cup): Flammable gas. Ignites spontaneously in moist air.
Flammable Limits: LFL - 0.8%; UFL - 88%
Autoignition Temperature: 100-125°F/38-52°C

EXTINGUISHING MEDIA: Use water spray or fog.
DO NOT use halogenated extinguishing agents, since they may form shock sensitive mixtures with diborane.

UNUSUAL FIRE AND EXPLOSION HAZARDS: If a significant amount of diborane mixes with air in a restricted space before ignition takes place, delayed ignition will be explosive. Pure diborane is insensitive to mechanical shock, but shock and thermally sensitive mixtures may be formed in the presence of impurities such as oxygen and halogenated hydrocarbons. Mixing diborane with the chemicals listed in Section 10 can produce a fire or an explosion. Diborane burns with a green flame and produces a dense white smoke. Control, but do not extinguish, fire. Cool adjacent equipment. Shut off source, if possible. Allow fire to burn itself out. If it is necessary to extinguish fire, use water fog. Extinguishing fire without shutting off diborane source may lead to explosive reignition. Toxic residues may remain after fire.

To decontaminate area, hose down external surfaces and apply an aqueous solution containing 5% ammonia and 5% trisodium phosphate detergent.

PROTECTION OF FIRE FIGHTERS: Wear full protective clothing, including protective gloves and boots. For respiratory protection, wear a NIOSH approved self-contained breathing apparatus with full facepiece operated in a positive-pressure mode.

6. Accidental Release Measures

PROCEDURES FOR CLEANUP: Wear recommended personal protective equipment. Be prepared to fight fire. Eliminate ignition sources. Do not flush spill to drain. Mix with large amounts of DRY soda ash. Using non-sparking tools, scoop solids into a DRY metal container, properly label, and cover. Take immediately to a waste handling area. If contaminated, flammable hydrogen gas can evolve and cause fire, explosion, or pressure buildup in container. Properly dispose of all residues immediately. Handle in compliance with all local, state, and federal laws and regulations. The reportable quantity for diborane is 100 pounds.

7. Handling And Storage

HYGIENIC PRACTICES: Do not breathe vapor or mist. Use only with adequate ventilation. Keep container tightly closed. Do not get in eyes, on skin, or on clothing. Wash thoroughly after handling.
STORAGE: Store in noncombustible, well-ventilated structure away from heat, sparks, and flames. Refrigerate. Decomposition can be significantly reduced by storing at -20°C/-4°F or less. DO NOT store cylinders below -80°C/-112°F. DO NOT store cylinders in liquid nitrogen. Cylinder material becomes brittle when extremely cold. Handle and store in a DRY closed system under DRY nitrogen gas. Do not store residues. Properly dispose of all residues immediately.

SARA Section 302 requires notification to State Emergency Response Commission for storage or use at amounts greater than or equal to 100 pounds. SARA Section 302 requires facilities storing a TPQ substance to participate in local emergency response planning.

WORK PRACTICES: Keep away heat, sparks, flame and any possible contact with water, moist air, alcohols, acids, and other incompatible materials. Do not expose to air. Handle and store in a closed system under DRY nitrogen gas. Use non-sparking tools when opening or closing containers. Bond and ground all systems when handling. Since empty containers retain product residue, follow label warnings even after container is emptied.

Boric acid forms from exposure to moisture with subsequent powder coating of flow path components. During periods of inactivity, trapped gas degrades into higher boranes which clog bypass holes, sensors, and other component parts.

PROTECTIVE MEASURES DURING REPAIR AND MAINTENANCE OF CONTAMINATED EQUIPMENT: Do not attempt repair or maintenance of contaminated equipment until it has been cleaned. Ventilate area. Eliminate ignition sources.

Transfer residual diborane and purge system with dry nitrogen, flaring or scrubbing gases. A three-step cleaning process is used to remove any remaining diborane. First, use DRY naphtha. After removing it, slowly add isopropanol, venting any hydrogen gas produced. After removing the isopropanol, slowly add methanol venting any hydrogen gas. All washout solutions should be tightpiped to drums and handled as toxic. Take immediately to a waste handling area. If contaminated, flammable hydrogen gas can evolve and cause fire, explosion, or pressure buildup in container. Properly dispose of all residues immediately.

8. Exposure Controls/Personal Protection

ENGINEERING CONTROLS: Maintain a leakproof system. Use packless valves, welded piping, and other leakproof construction. Handle in a closed system under DRY nitrogen gas. Provide adequate local exhaust ventilation to maintain worker exposure below exposure limits. Prevent electrostatic charge buildup by using common bonding and grounding techniques. Use DRY nitrogen gas to inert containers, transfer lines, vessels, tanks, etc., such that the atmosphere stays below 3% oxygen.

EXPOSURE CONTROLS: None established for the mixture.
For diborane:  
OSHA PEL-TWA: 0.1 ppm (0.1 mg/m³)
ACGIH TLV-TWA: 0.1 ppm
The IDLH for diborane is 15 ppm.

The median detectable concentration (MDC) of diborane in air for humans was determined to be 3.7 mg/m³ or 3.2 ppm, with a range of 0.2 - 6 mg/m³. (Comstock, C. C. and F. W. Oberst: The Median Detectable Concentration of Diborane, Pentaborane, and Decaborane by Odor for Man, Army Chemical Corps Medical Laboratories, Research Report #206, August 1, 1953.)

PERSONAL PROTECTIVE EQUIPMENT:
Normal Use & Handling: When exposure to eyes and skin is possible, wear chemical protective goggles with a faceshield and flame-retardant protective clothing. Very limited glove permeation data exists for this product: Butyl rubber gloves are NOT recommended based on degradation occurring in less than one hour. Exposure limits have been established for diborane. When inhalation of unknown concentrations of diborane vapor or mist is possible, wear a NIOSH-approved self-contained breathing apparatus with full facepiece operated in a positive-pressure mode. NIOSH recommendations for respirator selection and maximum concentration for use (MUC) are listed below:

<table>
<thead>
<tr>
<th>Condition</th>
<th>Minimum Respiratory Protection (required above 0.1 ppm)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Up to 1 ppm (APF = 10)</td>
<td>Any supplied-air respirator.</td>
</tr>
<tr>
<td>Up to 2.5 ppm (APF = 25)</td>
<td>Any supplied-air respirator operated in a continuous-flow mode.</td>
</tr>
<tr>
<td>Up to 5 ppm (APF = 50)</td>
<td>Any supplied-air respirator that has a tight-fitting facepiece and is operated in a</td>
</tr>
</tbody>
</table>
9. Physical And Chemical Properties

APPEARANCE: Colorless gas at room temperature. Liquid diborane is colorless.

ODOR: Irritating, sickly sweet, unpleasant, distinctive odor.

BOILING POINT @ 760 mm Hg: -134°F/-92.5°C
FREEZING POINT: -265°F/-165.5°C

VAPOR DENSITY: 0.952 @ 32°F/0°C
VAPOR PRESSURE @ -40°F/-40°C: 132 psia

DENSITY, SOLID @ -297°F/-183°C: 0.577 gm/cc; 36.02 lb/ft³
DENSITY, LIQUID @ -134°F/-92.5°C: 0.437 gm/ml; 3.64 lbs/gal

CRITICAL TEMPERATURE: 16.7°C
CRITICAL PRESSURE: 581 psia (39.5 atmospheres)

HEAT OF VAPORIZATION @ -92.5°C: 3.41 kcal/mol

HEAT OF COMBUSTION: 31,370 BTU/lb.

SOLUBILITY: Reacts rapidly with water and alcohols generating flammable hydrogen gas; soluble without reaction in dry hydrocarbons such as pentane and hexane; soluble in halogenated solvents but may form shock sensitive mixtures.

MOLECULAR WEIGHT: 27.68
FORMULA: B₂H₆

10. Stability And Reactivity

STABILITY (CONDITIONS TO AVOID): Stable. Keep away from heat, sparks, and flame. May decompose explosively above 40°C. Diborane polymerizes at room temperature, producing higher boron hydrides and hydrogen and increasing the pressure in the container.

INCOMPATIBILITY (SPECIFIC MATERIALS TO AVOID): Air, halogenated hydrocarbons, oxidizers, reactive metals (for example, lithium, aluminum; which form hydrides which may ignite spontaneously), chlorine, nitric acid, nitrogen trifluoride, phosphorous trifluoride, dimethyl sulfoxide, tetra vinyl lead, and sodium hydroxide + octanal oxime in tetrahydrofuran. Diborane will attack some forms of plastics, rubber, and coatings.

HAZARDOUS DECOMPOSITION PRODUCTS: Hydrogen, boron oxides

HAZARDOUS POLYMERIZATION: Can occur at room temperature. Produces higher boron hydrides and hydrogen.

11. Toxicological Information
Diborane is a gas that is toxic by inhalation, may cause eye irritation, and may cause central nervous system effects. Diborane gas acts primarily as an irritant to the respiratory system. Symptoms of acute exposure are respiratory distress, chest tightness, precordial pain, difficulty in breathing, non-productive coughing and wheezing, nausea, nervousness, dizziness, chest pain, shortness of breath, abdominal cramps, muscle fasciculations, and diarrhea. Symptoms appear within a few minutes. In cases of mild exposure, they may last less than an hour; in more severe exposures, generally three to five days. Secondary infections were reported in some persons needing treatment. Chronic respiratory distress was present in two persons from recurring diborane exposure; it was believed to be due to a hypersensitivity reaction.

Exposure to low concentrations of diborane over a prolonged time period can cause lightheadedness, headache, fatigue, drowsiness, tremors, vertigo, chills, and sometimes fever; a cough and chest tightness may be present. Symptoms lasted from five days to three weeks.

Since the detectable concentration is above the exposure limit and diborane offers no other warning properties (such as eye irritation) around the exposure limit, diborane should be treated as a chemical with poor warning properties. The odor of diborane is unique and offers some limited warning, but potentially hazardous concentrations which cannot be detected by smell can exist in air. The median detectable concentration (MDC) of diborane in air for humans was determined to be 3.7 mg/m3 or 3.2 ppm, with a range of 0.2 - 6 mg/m3. In addition, prolonged exposure to diborane can temporarily impair the sense of smell.

Laboratory animals exposed to large acute or subacute doses sustained some kidney and liver damage, but none was found in animals exposed to relatively small chronic doses. No permanent damage was found in exposed workers.

Diborane was an in vitro mutagen (Salmonella typhi with and without S9 activation) at very high concentrations (2000 ppm and 5000 ppm).

TOXICITY DATA:
- LC50 (rat-inhalation): 40 ppm, 4 hours
- LC50 (mouse-inhalation): 29 ppm, 4 hours
- LCLo (dog-inhalation): 125 ppm, 2 hours
- LCLo (hamster-inhalation): 50 ppm, 8 hours

12. Ecological Information

ECOLOGICAL DATA: No environmental toxicity data for the product.

13. Disposal Considerations

WASTE DISPOSAL: Do not flush to sewer. Dispose in compliance with all local, state, and federal laws and regulations.

14. Transport Information

Refrigerated diborane is shipped using DOT Exemption, DOT-E 970.

Note: The reportable quantity (RQ) for diborane is 100 pounds.

Diborane is TOXIC - INHALATION HAZARD, ZONE A.

HAZARDOUS MATERIALS/DANGEROUS GOODS CLASSIFICATION:
- Proper Shipping Name: Diborane, compressed
- Hazard Class: 2.3 (Subsidiary risk class - 2.1)
- Packaging Group: Not applicable
- Identification Number: UN1911
- Labels: Poison gas (inhalation hazard) and flammable gas

15. Regulatory Information

TSCA: Diborane listed on the TSCA Public Inventory.

SARA 313 INFORMATION: Diborane does not contain a toxic chemical or chemicals subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR 372.

CERCLA/SUPERFUND: The reportable quantity (RQ) for diborane is 100 pounds.

EINECS: 242-940-6 for diborane
EUROPEAN LABEL INFORMATION:
Symbols: F+, T, Xi
Indications of danger (Annex II): Extremely flammable, Toxic, and Irritant
Nature of special risk attributed to dangerous substances (Annex III):
- R12 Extremely flammable.
- R23 Toxic by inhalation.
- R36/38 Irritating to eyes and skin.
Safety advice concerning dangerous chemical substances (Annex IV):
- S24/25 Avoid contact with skin and eyes.
- S26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
- S35 This material and its container must be disposed of in a safe way.
- S36 Wear suitable protective clothing.
- S45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
- S46 If swallowed, seek medical advice immediately and show this container or label.

CANADA: This product contains diborane, a chemical listed on the WHMIS Ingredient Disclosure List.

CALIFORNIA: This product does not contain a chemical known to the State of California to cause cancer.

NEW JERSEY: This product contains diborane a chemical listed on the New Jersey Department of Health Hazard Right-to-Know Program Hazardous Substance List as a special health hazard.

PENNSYLVANIA: This product contains diborane and is subject to the Pennsylvania Worker and Community Right-to-Know Act.

16. Other Information

WARNING: This is a dangerous chemical product. By following the directions and warnings provided with this product, the dangers associated with the use of this product can be greatly reduced but never entirely eliminated. Callery Chemical Company makes no warranties, expressed or implied, with respect to this product and EXPRESSLY DISCLAIMS THE WARRANTY OF MERCHANTABILITY AND ANY WARRANTY OF FITNESS FOR A PARTICULAR PURPOSE. Users assume all risks in handling, using or storing this product.

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