Hexachlorobutadiene
87–68–3

Hazard Summary

Hexachlorobutadiene is used mainly as an intermediate in the manufacture of rubber compounds. No information is available on the health effects of hexachlorobutadiene in humans. Animal studies have reported effects on the kidney and respiratory system from acute inhalation exposure, and effects on the kidney from chronic oral exposure to hexachlorobutadiene. Animal studies have not reported developmental or reproductive effects, other than a reduction in fetal body weights, from inhalation exposure to hexachlorobutadiene. One study reported kidney tumors in rats exposed to hexachlorobutadiene orally. EPA has classified hexachlorobutadiene as a Group C, possible human carcinogen.

Please Note: The main sources of information for this fact sheet are EPA’s Integrated Risk Information System (IRIS) (3), which contains information on the carcinogenic effects of hexachlorobutadiene including the unit cancer risk for inhalation exposure, and the Agency for Toxic Substances and Disease Registry’s (ATSDR’s) Toxicological Profile for Hexachlorobutadiene. (1)

Uses

- Hexachlorobutadiene is used mainly as an intermediate in the manufacture of rubber compounds. It is also used in the production of lubricants, as a fluid for gyroscopes, as a heat transfer liquid, and in hydraulic fluids. (1)

Sources and Potential Exposure

- Average concentrations of hexachlorobutadiene in ambient air were reported to be around 0.003 parts per billion (ppb), while much higher levels (0.022 to 43 ppb) were reported near industries where hexachlorobutadiene is formed or used. (1)
- Very small amounts of hexachlorobutadiene may be present in drinking water (<1 ppb). (1)
- Levels of hexachlorobutadiene ranging from 0.1 to 4.7 milligrams per kilogram (mg/kg) have been found in fish. (1)
- Persons working in industries where hexachlorobutadiene is formed or used may be exposed to the chemical. (1)

Assessing Personal Exposure

- Hexachlorobutadiene or its breakdown products can be measured in urine or fat for several days after the exposure has occurred. (1)

Health Hazard Information

Acute Effects:

- No information is available regarding the acute (short-term) effects of hexachlorobutadiene in humans from inhalation or oral exposure. (1)
- Animal studies have reported effects on the kidney and respiratory system from acute inhalation exposure,
while oral animal studies have reported kidney effects. (1) Tests involving acute oral and inhalation exposures of rats and mice have shown hexachlorobutadiene to have high acute toxicity. (2)

**Chronic Effects (Noncancer):**
- No information is available regarding the chronic (long-term) effects of hexachlorobutadiene in humans from inhalation or oral exposure. (1)
- Animal studies have reported effects on the kidney and liver from chronic oral exposure to hexachlorobutadiene. (1)
- EPA has not established a Reference Concentration (RfC) for hexachlorobutadiene. (3)
- The California Environmental Protection Agency (CalEPA) has calculated a chronic inhalation reference exposure level of 0.09 milligrams per cubic meter (mg/m$^3$) for hexachlorobutadiene. The CalEPA reference exposure level is a concentration at or below which adverse health effects are not likely to occur. It is not a direct estimator of risk but rather a reference point to gauge the potential effects. At lifetime exposures increasingly greater than the reference exposure level, the potential for adverse health effects increases. (6)
- The Reference Dose (RfD) for hexachlorobutadiene is under review by EPA. (3)
- EPA has calculated a provisional RfD of 0.0002 milligrams per kilogram body weight per day (mg/kg/d) based on kidney effects in mice. The provisional RfD is a value that has had some form of Agency review but is not on IRIS. The RfD is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious noncancer effects during a lifetime. (4)

**Reproductive/Developmental Effects:**
- No information is available regarding the developmental or reproductive effects of hexachlorobutadiene in humans. (1)
- One study reported that the frequency of abnormal sperm morphology did not increase significantly over controls in mice exposed to hexachlorobutadiene via inhalation. A study in rats exposed via inhalation reported no embryotoxic effects, except for a reduction in fetal body weights. (1)
- Oral animal studies have reported reduced fertility, reduced fetal body weights, but no birth defects or other developmental effects from hexachlorobutadiene exposure. (1)

**Cancer Risk:**
- No information is available regarding the carcinogenic effects of hexachlorobutadiene in humans or animals from inhalation exposure. (1)
- One study reported kidney tumors in rats exposed to hexachlorobutadiene orally. (1,3)
- EPA has classified hexachlorobutadiene as a Group C, possible human carcinogen. (3)
- EPA uses mathematical models, based on animal studies, to estimate the probability of a person developing cancer from breathing air containing a specified concentration of a chemical. EPA calculated an inhalation unit risk estimate of $2.2 \times 10^{-5}$ (µg/m$^3$). EPA estimates that, if an individual were to continuously breathe air containing hexachlorobutadiene at an average of $0.05 \mu g/m^3$ (5 x $10^{-5}$ mg/m$^3$) over his or her entire lifetime, that person would theoretically have no more than a one-in-a-million increased chance of developing cancer as a direct result of breathing air containing this chemical. Similarly, EPA estimates that breathing air containing 0.5 µg/m$^3$ (5 x $10^{-4}$ mg/m$^3$) would result in not greater than a one-in-a-hundred thousand increased chance of developing cancer, and air containing 5.0 µg/m$^3$ (5 x $10^{-3}$ mg/m$^3$) would result in not greater than a one-in-ten-thousand increased chance of developing cancer. For a detailed discussion of confidence in the potency estimates, please see IRIS. (3)
- EPA has calculated an oral cancer slope factor of 0.078 (mg/kg/d)$. (3)

**Physical Properties**
Hexachlorobutadiene is a colorless liquid with a turpentine-like odor. (5)
- The odor threshold for hexachlorobutadiene is 1 part per million (ppm). (1)
- The chemical formula for hexachlorobutadiene is C₆Cl₆, and the molecular weight is 260.76 g/mol. (1)
- The vapor pressure for hexachlorobutadiene is 0.15 mm Hg at 25 °C, and it has an octanol/water partition coefficient (log Kow) of 4.78. (1)

Conversion Factors (only for the gaseous form):
To convert concentrations in air (at 25 °C) from ppm to mg/m³: mg/m³ = (ppm) × (molecular weight of the compound)/(24.45). For hexachlorobutadiene: 1 ppm = 10.7 mg/m³. To convert concentrations in air from µg/m³ to mg/m³: mg/m³ = (µg/m³) × (1 mg/1,000 µg).

### Health Data from Inhalation Exposure

#### Hexachlorobutadiene

<table>
<thead>
<tr>
<th>Health numbers</th>
<th>Regulatory, advisory numbers</th>
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<tbody>
<tr>
<td>LC₅₀ (mL)</td>
<td>AIHA ERPG-2 (107 mg/m³)</td>
</tr>
<tr>
<td>NOAEL (107 mg/m³)</td>
<td>AIHA ERPG-1 (32 mg/m³)</td>
</tr>
<tr>
<td>CalEPA chronic reference exposure level (100 mg/m³)</td>
<td>ACGIH TLV, NIOSH REL (0.24 mg/m³)</td>
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<tr>
<td>EPA Cancer Risk Level (10⁻⁶ excess lifetime risk = 5×10⁻⁶ mg/m³)</td>
<td>Ref. 7.8</td>
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**AIHA ERPG**—American Industrial Hygiene Association's emergency response planning guidelines. ERPG 1 is the maximum airborne concentration below which it is believed nearly all individuals could be exposed up to one hour without experiencing other than mild transient adverse health effects or perceiving a clearly defined objectionable odor; ERPG 2 is the maximum airborne concentration below which it is believed nearly all individuals could be exposed up to one hour without experiencing or developing irreversible or other serious health effects that could impair their abilities to take protective action.

**ACGIH TLV**—American Conference of Governmental and Industrial Hygienists' threshold limit value expressed as a
time-weighted average; the concentration of a substance to which most workers can be exposed without adverse effect.

\(\text{LC}_{50}\) (Lethal Concentration 50)---A calculated concentration of a chemical in air to which exposure for a specific length of time is expected to cause death in 50% of a defined experimental animal population.

NIOSH REL---National Institute of Occupational Safety and Health's recommended exposure limit; NIOSH-recommended exposure limit for an 8- or 10-h time-weighted-average exposure and/or ceiling.

The health and regulatory values cited in this factsheet were obtained in December 1999.

\(a\) Health numbers are toxicological numbers from animal testing or risk assessment values developed by EPA.

\(b\) Regulatory numbers are values that have been incorporated in Government regulations, while advisory numbers are nonregulatory values provided by the Government or other groups as advice. NIOSH, ACGIH, and AIHA numbers are advisory.

\(c\) These cancer risk estimates were derived from oral data and converted to provide the estimated inhalation risk.

\(d\) The NOAEL is from the critical study used as the basis for the CalEPA chronic reference exposure level.

References

Summary created in April 1992, updated January 2000


