

Hexachlorobutadiene; CASRN 87-68-3

Human health assessment information on a chemical substance is included in the IRIS database only after a comprehensive review of toxicity data, as outlined in the [IRIS assessment development process](#). Sections I (Health Hazard Assessments for Noncarcinogenic Effects) and II (Carcinogenicity Assessment for Lifetime Exposure) present the conclusions that were reached during the assessment development process. Supporting information and explanations of the methods used to derive the values given in IRIS are provided in the [guidance documents located on the IRIS website](#).

STATUS OF DATA FOR Hexachlorobutadiene

File First On-Line 01/31/1987

Category (section)	Assessment Available?	Last Revised
Oral RfD (I.A.)	withdrawn	05/01/1993
Inhalation RfC (I.B.)	not evaluated	
Carcinogenicity Assessment (II.)	yes	03/31/1987

I. Chronic Health Hazard Assessments for Noncarcinogenic Effects

I.A. Reference Dose for Chronic Oral Exposure (RfD)

Substance Name — Hexachlorobutadiene
CASRN — 87-68-3

The Oral RfD for hexachlorobutadiene has been withdrawn on 05/01/1993 as a result of further review.

Agency Work Group Review — 12/18/1985, 04/01/1993

EPA Contacts:

Please contact the IRIS Hotline for all questions concerning this assessment or IRIS, in general, at (202)566-1676 (phone), (202)566-1749 (FAX) or hotline.iris@epa.gov (internet address).

I.B. Reference Concentration for Chronic Inhalation Exposure (RfC)

Substance Name — Hexachlorobutadiene
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Not available at this time.

II. Carcinogenicity Assessment for Lifetime Exposure

Substance Name — Hexachlorobutadiene
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Last Revised — 03/31/1987

Section II provides information on three aspects of the carcinogenic assessment for the substance in question; the weight-of-evidence judgment of the likelihood that the substance is a human carcinogen, and quantitative estimates of risk from oral exposure and from inhalation exposure. The quantitative risk estimates are presented in three ways. The slope factor is the result of application of a low-dose extrapolation procedure and is presented as the risk per (mg/kg)/day. The unit risk is the quantitative estimate in terms of either risk per ug/L drinking water or risk per ug/cu.m air breathed. The third form in which risk is presented is a drinking water or air concentration providing cancer risks of 1 in 10,000, 1 in 100,000 or 1 in 1,000,000. The rationale and methods used to develop the carcinogenicity information in IRIS are described in The Risk Assessment Guidelines of 1986 (EPA/600/8-87/045) and in the IRIS Background Document. IRIS summaries developed since the publication of EPA's more recent Proposed Guidelines for Carcinogen Risk Assessment also utilize those Guidelines where indicated (Federal Register 61(79):17960-18011, April 23, 1996). Users are referred to Section I of this IRIS file for information on long-term toxic effects other than carcinogenicity.

II.A. Evidence for Human Carcinogenicity

II.A.1. Weight-of-Evidence Characterization

Classification — C; possible human carcinogen

Basis — Observation of renal neoplasms in male and female rats in one study

II.A.2. Human Carcinogenicity Data

None.

II.A.3. Animal Carcinogenicity Data

Groups of 39 or 40 Sprague-Dawley rats/sex/dose were maintained on diets formulated to deliver 0.2, 2 or 20 mg hexachlorobutadiene/kg bw/day. High-dose group males experienced significant increases in mortality. At the end of the 22- or 24-month study period, renal tubular adenomas and carcinomas had developed in 18% of high-dose females. There was no significant increase in incidence of neoplasms at other sites (Kociba et al., 1977).

Hexachlorobutadiene did not induce pulmonary adenomas in strain A mice treated via i.p. injection (Theiss, 1977).

II.A.4. Supporting Data for Carcinogenicity

Hexachlorobutadiene is not mutagenic for *Salmonella typhimurium* with or without the addition of rat liver homogenates (Taylor, 1978).

II.B. Quantitative Estimate of Carcinogenic Risk from Oral Exposure

II.B.1. Summary of Risk Estimates

Oral Slope Factor — $7.8E-2$ per (mg/kg)/day

Drinking Water Unit Risk — $2.2E-6$ per (ug/L)

Extrapolation Method — Linearized multistage procedure, extra risk

Drinking Water Concentrations at Specified Risk Levels:

Risk Level	Concentration
E-4 (1 in 10,000)	$5E+1$ ug/L
E-5 (1 in 100,000)	$5E+0$ ug/L

Risk Level	Concentration
E-6 (1 in 1,000,000)	5E-1 ug/L

II.B.2. Dose-Response Data (Carcinogenicity, Oral Exposure)

Tumor Type — renal tubular adenomas and adenocarcinomas

Test Animals — rat, Sprague-Dawley, male

Route — diet

Reference — Kociba et al., 1977

Administered Dose (mg/kg)/day	Human Equivalent Dose (mg/kg)/day	Tumor Incidence
0	0	1/90
0.2	0.04	0/40
2.0	0.4	0/40
20.0	4.0	9/39

II.B.3. Additional Comments (Carcinogenicity, Oral Exposure)

Test material was 99% pure. Concentrations in diet were adjusted to deliver the above dosages. To obtain equivalent human doses, a rat lifetime of 770 days and a weight of 0.610 kg were assumed.

The unit risk should not be used if the water concentration exceeds 5E+3 ug/L, since above this concentration the unit risk may not be appropriate.

II.B.4. Discussion of Confidence (Carcinogenicity, Oral Exposure)

There were sufficient numbers of animals tested and there was a significant increase in tumor incidence by comparison to concurrent controls.

II.C. Quantitative Estimate of Carcinogenic Risk from Inhalation Exposure

II.C.1. Summary of Risk Estimates

Inhalation Unit Risk — 2.2E-5 per (ug/cu.m)

Extrapolation Method — Linearized multistage procedure, extra risk

Air Concentrations at Specified Risk Levels:

Risk Level	Concentration
E-4 (1 in 10,000)	5E+0ug/cu.m
E-5 (1 in 100,000)	5E-1 ug/cu.m
E-6 (1 in 1,000,000)	5E-2 ug/cu.m

II.C.2. Dose-Response Data for Carcinogenicity, Inhalation Exposure

The inhalation risk estimates were calculated from the oral exposure data in Section II.B.2.

II.C.3. Additional Comments (Carcinogenicity, Inhalation Exposure)

The unit risk should not be used if the air concentration exceeds 5E+2 ug/cu.m, since above this concentration the unit risk may not be appropriate.

II.C.4. Discussion of Confidence (Carcinogenicity, Inhalation Exposure)

See II.B.4.

II.D. EPA Documentation, Review, and Contacts (Carcinogenicity Assessment)

II.D.1. EPA Documentation

Source Document — U.S. EPA, 1980

The 1980 Ambient Water Quality Criteria Document for Hexachlorobutadiene received Agency and peer review.

II.D.2. EPA Review (Carcinogenicity Assessment)

Agency Work Group Review — 11/12/1986

Verification Date — 11/12/1986

II.D.3. EPA Contacts (Carcinogenicity Assessment)

Please contact the IRIS Hotline for all questions concerning this assessment or IRIS, in general, at (202)566-1676 (phone), (202)566-1749 (FAX) or hotline.iris@epa.gov (internet address).

III. [reserved]

IV. [reserved]

V. [reserved]

VI. Bibliography

Substance Name — Hexachlorobutadiene
CASRN — 87-68-3

VI.A. Oral RfD References

Not available at this time

VI.B. Inhalation RfC References

None

VI.C. Carcinogenicity Assessment References

Kociba, R.J., D.G. Keyes, G.C. Jersey, et al. 1977. Results of a two-year chronic toxicity study with hexachlorobutadiene in rats. *Am. Ind. Hyg. Assoc. J.* 38: 589-602.

Taylor, G. 1978. Personal communication. National Institute of Occupational Safety and Health, Cincinnati, OH. (Cited in U.S. EPA, 1980)

Thiess, J.C., G.D. Stoner, M.B. Shimkin and E.K. Weisburger. 1977. Test for carcinogenicity of organic contaminants of United States drinking waters by pulmonary tumor response in strain A mice. *Cancer Res.* 37: 2717-2720.

U.S. EPA. 1980. Ambient Water Quality Criteria Document for Hexachloro- butadiene. Prepared by the Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH for the Office of Water Regulations and Standards, Washington, DC. EPA 440/5-80-053. NTIS PB 81-117640.

VII. Revision History

Substance Name — Hexachlorobutadiene
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Date	Section	Description
03/31/1987	II.	Carcinogenicity Section added
05/01/1993	I.A.	Withdrawn

VIII. Synonyms

Substance Name — Hexachlorobutadiene
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Last Revised — 01/31/1987

- 87-68-3
- 1,3-Butadiene, Hexachloro-
- DOLEN-PUR
- GP-40-66:120
- HCBBD
- Hexachlor-1,3-Butadien
- HeXachlorbutadiene
- Hexachlorobutadiene
- 1,1,2,3,4,4-Hexachloro-1,3-Butadiene
- 1,3- Hexachlorobutadiene
- Perchlorobutadiene
- RCRA Waste Number U128
- UN 2279