

GDCh-Advisory Committee
on Existing Chemicals (BUA)

p-Chlorobenzyl chloride

BUA Report 236

(February 2002)



S. Hirzel

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on Existing Chemicals (BUA, Status February 2002)

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für Altstoffe (BUA)



S. Hirzel

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Preface

The Advisory Committee on Existing Chemicals of Environmental Relevance, BUA for short, was established in May 1982 to help the German federal government cope with the large task of dealing with existing chemicals. In an agreement between federal government, scientific community, and the chemical industry, it was associated with the German Chemical Society (GDCh, Gesellschaft Deutscher Chemiker) to ensure objective work carried out in accordance with scientific principles. Since the beginning of 2001 the BUA has been composed of scientists from the research areas of chemistry, analytics, monitoring, toxicology, primary and secondary exposition, aquatic and terrestrial toxicology as well as the fate and behaviour of compounds in water, soil, air. The BUA is supported by experts from federal government agencies and the German Chemical Industry Association (VCI, Verband der Chemischen Industrie).

No other national or international body has dealt with the ecological and health-related effects of as many existing chemicals as the BUA. Upon the recommendation of the federal government, the BUA has participated as a Peer-Review Group in the evaluation of ICCA-compounds (ICCA, International Council of Chemical Associations) since 2000 and also acts as the Contact Point in the OECD-HPV-Chemicals Programme (High Production Volume). The goal of the initiative is on the one hand to complete the data on the HPV chemicals and on the other to undertake an internationally coordinated evaluation of their hazard potential.

The BUA began an additional national project in 1997, which also selects and assesses existing chemicals with a lower production volume in the range of 100 - 1000 tonnes/year. The chemical industry presents about 50 datasets for such substances each year, for which the BUA sets the priority. Comprehensive reports are published on chemicals suspected of having a hazard potential. If the data available for substance assessment are insufficient, the gaps in knowledge are documented and, if necessary, investigations recommended. On the national level, the BUA has produced comprehensive reports on about 330 substances and carried out preliminary evaluation and classification (priority-setting) for approximately 200 more. The processes leading to priority-setting and the BUA reports are published to lend transparency to the Committee's work.

Moreover, BUA is increasingly addressing scientific questions and problems, which apply simultaneously to many compounds, among others: "Marine Risk Assessment: Concept and Criteria" (BUA Report 220), "Biological Impact of Synthetic and Natural Endocrine Active Substances – Effects on Human Health" (BUA Report 228), Risk Assessment of Substances in Soils" (BUA Report 230), "Persistent Organic Pollutants (POPs)" (BUA Report 232) and "Safety Factors in Toxicological Risk Assessment". For each of these themes an analysis is made of the scientific state of the art, is documented and the results published in reports such as the current volume. The aim of BUA is to develop assessment concepts, determine data gaps, point out the need for further research and, last but not least, also to reduce information deficits in the general population.

Weihenstephan
February, 2002

Helmut Greim
BUA Chairman

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Abbreviations

BCF	Bioconcentration Factor
BP	Boiling Point
bw	body weight
CAS	Chemical Abstracts Service
CBC	Chlorobenzylchloride
DL	Detection Limit
DOC	Dissolved Organic Carbon
EC	Effect Concentration
ECD	Electron Capture Detection
EINECS	European Inventory of Existing Chemical Substances
FID	Flame Ionization Detector
FTIR	Fourier Transformation Infrared
GC	Gas Chromatography
HPLC	High Performance Liquid Chromatography
IR	Infrared
IUCLID	International Uniform Chemical Information Database
MS	Mass Spectroscopy
t	tonne(s)
TGD	Technical Guidance Documents
ThOD	Theoretical Oxygen Demand
yr	year

BUA Report on p-Chlorobenzyl chloride

Summary

Ecological Aspect

The only known producer of p-chlorobenzyl chloride in Europe in 2000 was the firm Clariant GmbH which produced 450 t/yr in Germany. In Japan, over 1000 t p-chlorobenzyl chloride/yr are produced by the firm Ihara and processed nationally by the mother company.

About 350 t of the annual production of p-chlorobenzyl chloride at Clariant GmbH are further processed within Germany by Bayer AG at the Dormagen site; 100 t are sold mainly outside of Europe.

p-Chlorobenzyl chloride is used as an intermediate chiefly for synthesizing active ingredients in the agrochemical field; a small fraction is also used in the pharmaceutical sector.

At Bayer AG about 100 t/yr are reacted to a chemical intermediate that is completely sold to one customer in Western Europe; 200 – 400 t/yr (annual deviations) are processed to a fungicide active ingredient.

No p-chlorobenzyl chloride enters the environment during production (Clariant GmbH) or processing (Bayer AG). The resulting products of Bayer AG show no residual contents of p-chlorobenzyl chloride.

There are no data available on the further processing of 100 t which are exported mostly outside of Europe.

There is no information available on imports.

p-Chlorobenzyl chloride is not a component of formulations used for consumer products.

At a German production site, p-chlorobenzyl chloride is formed as a by-product of the continuous gas-phase chlorination of toluene. It is found in a concentration of 6 – 26 mg/l in raw wastewater. After biological wastewater treatment, the concentration is less than 5 – 5.7 µg/l.

There are no data available about its occurrence in the environment.

According to an insufficiently documented Zahn-Wellens test, p-chlorobenzyl chloride is inherently degradable.

p-Chlorobenzyl chloride is hydrolyzed in water to p-chlorobenzylalcohol. On the basis of older studies on the hydrolysis rate, p-chlorobenzyl chloride has a half-life of 41 – 47 hours upon hydrolysis at neutral pH and a temperature of 20 °C. The rate of hydrolysis increases with pH value and temperature.

Corresponding to its behavior in water, p-chlorobenzyl chloride is hydrolyzed in soils upon contact to moisture. A statement cannot be made on the respective half-life.

p-Chlorobenzyl chloride is photochemically degraded in air by OH-radicals, whereby the calculated half-life is 309 hours ($5 \cdot 10^5$ OH-radicals/cm³). Because of its absorption properties for UV-light, the substance presumably is not directly degraded by photolysis.

Despite the log K_{OW} of 3.18, a potential for bioaccumulation of p-chlorobenzyl chloride can be excluded only provided that it makes contact to water and is thereby subjected to hydrolysis.

According to the classification scheme of Blume and Ahlsdorf (1993), p-chlorobenzyl chloride, with a log K_{OC} 2.68, has a moderate soil adsorption potential. Nonetheless, the hydrolyzability of the substance was not considered here.

The Henry's Law constant lies in the range of 26 – 155 Pa · m³/mol (without accounting for hydrolysis).

According to a Mackay Level I calculation, air is the target compartment of the equilibrium distribution of p-chlorobenzyl chloride (because of hydrolysis, this statement applies only for hours up to a few days).

An incompletely documented 24h test with *Daphnia magna* in a closed system yields an EC₅₀ value of 4.4 mg/l.

For *Leuciscus idus*, the 96h LC₀ and LC₁₀₀ value is 2 mg/l and 2.5 mg/l, respectively. The p-chlorobenzyl chloride concentration is not analytically monitored in the test in an open system (limited validity).

Studies on the hydrolysis product p-chlorobenzylalcohol:

According to two 24h tests (cannot be validated, no documentation) with *Daphnia magna* (DIN 38 412) and hydrolyzed p-chlorobenzyl chloride, the EC₅₀ values are 44.2 mg/l and 60 mg/l.

According to two insufficiently documented ETAD fermentation tube tests with hydrolyzed p-chlorobenzyl chloride, the 24h damage threshold is 38 – 41 mg/l.

Toxicological Aspect

Studies are not available on the metabolism and mode of action of p-chlorobenzyl chloride. p-Chlorobenzyl chloride is slightly toxic after acute oral or dermal application. There are no valid studies on the repeated application of p-chlorobenzyl chloride. In the mouse, p-chlorobenzyl chloride is shown to be strongly irritating to the respiratory tract. It is slightly irritating to the skin and eyes of rabbits. The substance is sensitizing in animal tests. p-Chlorobenzyl chloride is non-mutagenic in various strains of *Salmonella typhimurium* as well as in *E. coli* WP2 uvrA. A micronucleus test, cited as positive by the authors, cannot be evaluated because of serious methodical and documental deficiencies. Other studies on the genotoxicity in vitro and carcinogenicity are unavailable. There are no valid data on genotoxicity in vivo or toxic effect on reproduction.