

GDCh-Advisory Committee  
on Existing Chemicals (BUA)

## **4-tert-Butylbenzaldehyde**

BUA Report 224  
(June 2000)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2001

## **GDCh-Advisory Committee on Existing Chemicals (BUA, June 2000)**

### **Chairman:**

Prof. Dr. H. GREIM, GSF – Institut für Toxikologie, Oberschleißheim

### **Members:**

Prof. Dr. H. DREXLER, Institut für Arbeits-, Sozial- und Umweltmedizin der Universität Erlangen

Prof. Dr. Dr. H. GELBKE, BASF AG, Toxikologie, Ludwigshafen am Rhein

Frau Prof. Dr. U. GUNDERT-REMY, Bundesinstitut für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin

Dr. H. von HOLLEBEN, Verband der Chemischen Industrie, Frankfurt am Main

Prof. Dr. H. HULPKE, Bayer AG, Konzernstab KS-QUS, Leverkusen

Priv.-Doz. Dr. Dr. A. KAPPOS, Behörde für Arbeit, Gesundheit und Soziales der Freien Hansestadt Hamburg

Dr. J. KUTSCHER, Berufsgenossenschaft der Chemischen Industrie, Heidelberg

Dr. C. MEICHSNER, InfraServ GmbH & Co Höchst KG, Umwelt/Sicherheit, Frankfurt/Main

Prof. Dr. R. NAGEL, Institut für Hydrobiologie der Technischen Universität Dresden

Dir. und Prof. Dr. H. NEIDHARD, Umweltbundesamt, Berlin

Dr. N. RUPPRICH, Bundesanstalt für Arbeitsschutz und Arbeitsmedizin, Dortmund

Prof. Dr. R. ZELLNER, Institut für Physikalische und Theoretische Chemie der Universität Essen (Vice Chairman)

### **Collaborators and Guests:**

Priv.-Doz. Dr. J. AHLERS, Fachgebiet IV 1.2 des Umweltbundesamtes, Berlin

Dr. T. BROCK, Berufsgenossenschaft der Chemischen Industrie, Heidelberg

Dr. F. ENDRES, BUA-Büro Essen

Dr. S. ETTTEL, BUA-Büro Essen

Dr. D. FINK, Verband der Chemischen Industrie, Frankfurt am Main

Dr. H. FLEIG, BASF AG, Toxikologie, Ludwigshafen am Rhein

Dr. E. GOEDECKE, Anmeldestelle Chemikaliengesetz, Dortmund

Frau Dr. H. GREIM, BUA-Büro München

Dr. G.-R. JÄNIG, Fachgebiet 821 des Bundesinstituts für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin

MinR Dr. H. A. KLEIN, Bundesministerium für Arbeit und Sozialordnung, Bonn

Frau Dipl.-Ing. S. KNIESTEDT, BASF AG, Ludwigshafen am Rhein

Dr. J. KOPPENHÖFER, BUA-Büro Essen

Dr. W. KÖRDEL, Institut für Umweltchemie und Ökotoxikologie der Fraunhofer-Gesellschaft, Schmallenberg

Frau Dr. P. KREIS, BUA-Büro München

Frau Dr. M. LANGE, Institut für Hydrobiologie der Technischen Universität Dresden

Frau Dr. C. POHLENZ-MICHEL, BUA-Büro München

Frau Dipl.-Biol. L. WEIS, BUA-Büro Essen

Frau Dr. K. WIDMANN, BUA-Büro München

Frau Dr. K. ZIEGLER-SKYLAKAKIS, BUA-Büro München

### **Responsible at the BMU:**

MinR Prof. Dr. U. SCHLOTTMANN, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, Bonn

### **GDCh-Office:**

Dr. H. BEHRET, GDCh, Frankfurt am Main

# **4-tert-Butylbenzaldehyde**

BUA Report 224  
(June 2000)

edited by the GDCh-Advisory Committee  
on Existing Chemicals

GDCh-Beratergremium  
für Altstoffe (BUA)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2001

Dr. H. Behret  
Gesellschaft Deutscher Chemiker  
Postfach 90 04 40  
D-60444 Frankfurt am Main  
E-Mail: [boa@gdch.de](mailto:boa@gdch.de)  
Homepage: <http://www.gdch.de>

Responsible at the BMU:  
MinR Prof. Dr. U. Schlottmann  
BMU  
Postfach 12 06 29  
D-53048 Bonn  
E-Mail: [schlottmann.ulrich@bmu.de](mailto:schlottmann.ulrich@bmu.de)

The work for this publication was sponsored by the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit (BMU) / Federal Environmental Agency (Umweltbundesamt)) and the German Chemical Industry Association (Verband der Chemischen Industrie, VCI)

This book was carefully produced. Nevertheless, authors, editors and publisher do not warrant the information contained therein to be free of errors. Readers are advised to keep in mind that statements, data, illustrations, procedural details or other items may inadvertently be inaccurate.

The use of general descriptive names, trade names, trademarks, etc. in a publication, even if not specifically identified, does not imply that these names are not protected by the relevant law and regulations.

Die Deutsche Bibliothek – CIP-Einheitsaufnahme

4-tert-Butylbenzaldehyde / ed. by the GDCh Advisory Committee on Existing Chemicals. [Transl. by P. Karbe] – (June 2000). – Stuttgart : Hirzel ; Stuttgart : Wiss. Verl.-Ges., 2001  
(BUA Report ; 224)  
Dt. Ausg. u. d. T.: 4-tert.-Butylbenzaldehyd  
ISBN 3-7776-1137-9

All rights reserved. No part of this publication may be translated, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without permission in writing from the publisher.

© 2001 S. Hirzel Verlag, Birkenwaldstraße 44, 70191 Stuttgart

Printed on acid-free and low-chlorine paper.

Printing and binding: Druckpartner Rübemann GmbH, Hemsbach  
Printed in F.R. Germany

## 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.

At the end of 1997, the Committee was renamed 'GDCh Advisory Committee on Existing Chemicals' (abbreviation 'BUA' as before) and the statutes were revised to include EU level aspects of occupational safety for the handling of existing chemicals from then on. The collaboration with the Employment Accident Insurance Fund of the Chemical Industry (BG-Chemie), with its knowledge on workplace exposure and the toxicologic properties of chemicals, is a valuable addition to the BUA's know-how.

The cooperation between authorities, industry, and the scientific community, upon which the BUA is based, has proven worthwhile. No other national or international body has dealt with the ecological and health-related effects of so many existing chemicals as the BUA. On the national level, the BUA has produced comprehensive reports on about 300 substances and carried out preliminary evaluation and classification (priority-setting) for approximately 200 more, as of 1997. Publication of the process leading to priority-setting, in addition to the BUA Reports, lends transparency to the Committee's work.

Since the EU presently considers only those substances with a production volume of more than 1000 tonnes/year, 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 databases for substances each year, for which the BUA sets the priority. Comprehensive reports are published on chemicals suspected of having a hazardous potential. If the data available for substance assessment are insufficient, the gaps in knowledge are documented and, if necessary, investigations recommended.

Moreover, BUA is increasingly addressing scientific questions and problems such as "endocrine disruptors", selection criteria for "persistent organic pollutants" (POPs), "risk assessment and evaluation models for soils and sediments", "evaluation criteria for the marine sector" and "safety factors within the framework of toxicological risk assessment". 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.

Munich, November 1999

Helmut Greim  
BUA Chairman



## Contents

### 4-tert-Butylbenzaldehyde

List of Abbreviations	IX
Summary and Conclusions	XI
Data Gaps	XIV
<b>1 Characterization of the Substance</b>	<b>1</b>
1.1 Descriptions of the Substance	1
1.2 Chemical and Physical Properties	1
Composition of the Technical Product	1
Chemical Properties	2
Physical Properties	2
<b>2 Analysis</b>	<b>4</b>
<b>3 Production, Application, Disposal – Emission into the Environment</b>	<b>6</b>
3.1 Production	6
Methods	6
Manufacturers and Quantities	6
Import, Export	7
3.2 Applications	7
3.3 Emission into the Environment	8
Emission into the Environment Through Production and Processing	8
Emission into the Environment Through Application	8
Formation from Non-Secondary Products	10
Overview of the Emission into the Environment	11
<b>4 Environmental Occurrence</b>	<b>12</b>
4.1 Measurements	12
4.2 Estimation	12
Atmosphere	12
Hydrosphere	12
Geosphere	12
<b>5 Environmental Behavior</b>	<b>13</b>
5.1 Transformation, Degradation, and Degradation Products	13
Biodegradation	13
Transformation in Air	14
Transformation in Water	14
Transformation in Soil	14
Degradation Products	15
5.2 Partitioning Behavior and Transport Processes	15
Accumulation	15
Partitioning	16

<b>6</b>	<b>Ecotoxicity</b>	18
6.1	Effects on Aquatic Organisms	18
	Summary	18
	Microorganisms	19
	Algae	20
	Invertebrates	20
	Vertebrates	21
6.2	Effects on Other Organisms	21
	Plants	21
	Invertebrates	21
	Vertebrates	21
<b>7</b>	<b>Toxicity in Warm-Blooded Animals</b>	22
7.1	General Effects	22
7.2	Mode of Action	22
7.3	Metabolism and Toxicokinetics	22
7.4	Acute Toxicity	23
7.5	Skin and Mucous Membrane Tolerance	24
7.6	Sensitizing Effect	25
7.7	Subacute, Subchronic, and Chronic Toxicity	26
7.8	Genotoxicity	26
7.9	Carcinogenicity	28
7.10	Reproduction Toxicity	28
7.11	Other Effects	28
7.12	Human Cases	29
<b>8</b>	<b>Substance-Specific Legal Regulations</b>	30
<b>9</b>	<b>References</b>	31
<b>Appendix 1: Simple Treat Model (TGD 1996, TGD - Erratum 1997)</b>		1
<b>Appendix 2: IUCLID Data Set from BASF AG</b>		1-35

## Abbreviations

BP	boiling point
CAS	Chemical Abstracts Service
DS	dry substance
DOC	dissolved organic carbon
EINECS	European Inventory of Existing Chemical Substances
FID	flame ionization detector
GC	gas chromatography
HPLC	high performance liquid chromatography
IR	infrared
IUCLID	International Uniform Chemical Information Database
MS	mass spectroscopy
TA Luft	Technical Instructions for Air Pollution Control
TBB	4-tert-butylbenzaldehyde
TB-benzoic acid	4-tert-butylbenzoic acid
TC	thin-layer chromatography
TGD	Technical Guidance Documents
ThOD	theoretical oxygen demand
TSCA	Toxic Substances Control Act



## Summary

### **Ecological Aspect**

The sole European manufacturer, the BASF AG in Ludwigshafen, Germany, produces 2000 tonnes/year of tert-butylbenzaldehyde (TBB). Except for about 200 kg within 2-3 years, the entire production is further processed internally to a fragrance.

Introductions into the atmosphere through production and processing are below the reporting level of 25 kg/year.

Introductions into the factory wastewater through production and processing amount to 1.7 tonnes/year, of which 1.43 tonnes/year enter receiving waters according to a model calculation.

Data are not available on the residual content in the fragrance produced from TBB, or on its possible re-cleavage.

Unquantifiable amounts are formed through the use of sunscreens, due to photolysis of its main ingredient.

Unquantifiable amounts are released as a result of the sale, on a laboratory scale, of 200 kg within 2-3 years.

No measurements are available on the environmental occurrence.

According to a Zahn-Wellens test TBB is potentially degradable, mainly by abiotic processes. There are indications that TBB is adsorbed on sewage sludge.

A low bioaccumulation potential is expected, due to the calculated log BCF of 1.94.

According to the classification system of Blume and Ahlsdorf, TBB has a medium potential for soil sorption (calculated  $\log K_{OC}$  2.6).

Vaporization from water is “possibly significant” to “significant” according to the criteria of Thomas.

According to estimates on the environmental distribution under equilibrium conditions (Mackay I) air and, to a lesser extent, water are the target compartments of TBB.

Of the tests on ecotoxicity to microorganisms, a short-term respiration-inhibition test (industrial sewage sludge), with an  $EC_{20}$  of 60 mg/l, showed the highest sensitivity. Three other short-term respiration-inhibition tests gave values in the range of 130 to 780 mg/l.

The lowest effective concentration in a 72-hour growth-inhibition test on algae (*Scenedesmus subspicatus*) was an  $EC_{10}$  of 19 mg/l. The results of a screening test indicate a lower effective concentration ( $EC_{10}$  4.3 mg/l).

In a static 48-hour test on *Daphnia magna* the  $EC_{50}$  amounted to 0.7 mg/l (nominal concentration), the NOEC being 0.3 mg/l.

In a 96-hour test on the golden orfe (*Leuciscus idus*), the  $LC_{50}$  was 8 mg/l and the  $LC_0$  2 mg/l (both nominal concentrations).

## Toxicological Aspect

p-tert-Butylbenzaldehyde is metabolized to p-tert-butylbenzoic acid. Apart from this, no confirmed data on the metabolism are available. In general, the metabolism and toxicokinetics of p-tert-butylbenzaldehyde have not been adequately investigated.

Following acute oral uptake, both in pure form and as a suspension in rape oil, LD<sub>50</sub> values in the rat are between 500 and 1000 mg p-tert-butylbenzaldehyde/kg BW. No irritant effect on the skin has been shown for humans or in animal experiments. There was also no irritant effect of p-tert-butylbenzaldehyde on mucous membranes. Following repeated intradermal induction in the adjuvant test in guinea pigs, p-tert-butylbenzaldehyde was clearly sensitizing, whereas an epicutaneous induction treatment showed no signs of a sensitizing effect in humans or guinea pigs. Thus, a possible sensitization through skin contact can be assumed.

In a methodically inadequate study, no health problems were reported for 5 workers who had been exposed to p-tert-butylbenzaldehyde over a period of 6 months. Following a 5-day oral administration of p-tert-butylbenzaldehyde in an animal experiment, the testis was identified as target organ. The substance has not been sufficiently tested for its genotoxicity or carcinogenicity.

The testicular changes, already observed in rats after a 5-day administration, could indicate an adverse effect of p-tert-butylbenzaldehyde on fertility (NOEL of 12.5 mg/kg BW and day). In mice, guinea pigs and dogs the histologic testicular changes at a dose of 100 mg/kg BW and day were less pronounced than in the rat.

## **Data Gaps**

### **Ecological Aspect**

At present, it is not possible to assess the introduction of TBB into the environment through contamination of secondary products, due to a lack of information.

### **Toxicological Aspect**

Several toxicological endpoints have not been adequately clarified:

- Studies with long-term administration: identification of target organs and NOEL
- Reproduction toxicity:

Investigations on adverse effects on development

Clarification of the indications of an adverse effect on fertility

- Genotoxicity: Investigations are missing on clastogenicity
- Carcinogenicity

These investigations are of low priority, however, before definitive exposure data are available.

Consumer exposure to p-tert-butylbenzaldehyde as degradation product of 4-tert-butyl-4'-methoxydibenzoylmethane (BM-DBM), used in sunscreens, has not been clarified.