

GDCh-Advisory Committee  
on Existing Chemicals (BUA)

**3,7-Dimethyloctane-3-ol**

BUA Report 253

(September 2004)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2006

**GDCh-Advisory Committee  
on Existing Chemicals (BUA, Status 09/2004)**

**Chairman:**

Prof. Dr. H. GREIM, Technische Universität München, Weihenstephan

**Members:**

Frau Dr. M. BETH-HÜBNER, Berufgenossenschaft der Chemischen Industrie, Heidelberg

Prof. Dr. N. CASPERS, Bayer AG, BIS-SUA-PUA I, Leverkusen

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

Frau Prof. Dr. H. FOTH, Institut für Umwelttoxikologie, Universität Halle an der Saale

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

Dr. W. KÖRDEL, Fraunhofer-Gesellschaft, IME, Schmallenberg

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

Prof. Dr. Dr. H. PARLAR, Institut für Lebensmitteltechnologie und Analytische Chemie,  
Technische Universität München

Dr. M. SCHÜMANN, Arbeitsgruppe Epidemiologie der IMDM/Universitätsklinik Hamburg-  
Eppendorf und Behörde für Wissenschaft und Gesundheit (BWG)

Dr. B. STOCK, Bayer AG, BIS-SUA-PUA I, Leverkusen

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

**Guests:**

Frau Dr. A. BAMBAUER, Anmeldestelle Chemikaliengesetz, Dortmund

Frau Prof. Dr. U. GUNDELT-REMY, Fachgebiet 8, Bundesinstitut für Risikobewertung, Berlin

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

Dr. M. LULEI, Verband der Chemischen Industrie, Frankfurt am Main

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

Dr. K. STEINHÄUSER, Umweltbundesamt, Berlin

**With the collaboration of:**

Dr. F. ENDRES, Universität Duisburg-Essen

Frau Dipl.-Biol. U. FRANK, Umweltbundesamt, Berlin

Frau Dr. H. GREIM, Technische Universität München, Weihenstephan

Dr. G.-R. JÄNIG, Fachgebiet 8, Bundesinstitut für Risikobewertung, Berlin

Frau Dr. B. LAUBE, Hannover

Dipl.-Biol. O. LICHT, Institut für Hydrobiologie, Technischen Universität Dresden

Frau Dr. I. NEUMANN, Technische Universität München, Weihenstephan

Frau Dr. C. RADKE, BASF AG, GUP/CB, Ludwigshafen am Rhein

Dr. S. SCHULTE, BASF AG, GUP/CA, Ludwigshafen am Rhein

Frau Dr. K. WIDMANN, Technische Universität München, Weihenstephan

**Responsible at BMU:**

MinR Prof. Dr.A. BASLER, Bundesministerium für Umwelt, Naturschutz und Reaktorsicher-  
heit, Bonn

**GDCh Office:**

Dr. K. BEGITT, GDCh, Frankfurt am Main

# **3,7-Dimethyloctane-3-ol**

BUA Report 253  
(September 2004)

edited by the GDCh-Advisory Committee  
on Existing Chemicals

GDCh-Beratergremium  
für Altstoffe (BUA)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2006

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

Responsible at the BMU:  
MinR Prof. Dr. A. Basler  
BMU  
Postfach 12 06 29  
D-53048 Bonn  
E-Mail: [armin.basler@bmu.bund.de](mailto:armin.basler@bmu.bund.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.

**Bibliographic information published by the Deutsche Nationalbibliothek**

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at <http://dnb.d-nb.de>.

ISBN 3-7776-1476-9  
ISBN 978-3-7776-1476-2

Translated by P. Karbe.

© 2006 S. Hirzel Verlag, Stuttgart

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.

Printed on acid-free and low-chlorine paper.

Printing and binding: Druckpartner Rübelmann GmbH, Hemsbach  
Printed in Germany

## Preface

The Advisory Committee on Existing Chemicals, 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 (Verband der Chemischen Industrie [VCI]).

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, as a group of expert advisors, 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"(BUA Report 244). 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  
October, 2004

Helmut Greim  
BUA Chairman



## Contents

|                     |     |
|---------------------|-----|
| Abbreviations ..... | IX  |
| Summary .....       | XI  |
| Data Gaps.....      | XIV |

### 3,7-Dimethyloctane-3-ol (CAS No. 78-69-3]

|          |   |    |
|----------|---|----|
| <b>1</b> | <b>Characterization of 3,7-Dimethyloctane-3-ol</b> .....                            | 1  |
| 1.1      | Chemical Identity .....   | 1  |
| 1.2      | Composition of the Technical Product .....  | 1  |
| 1.3      | Chemical and Physical Properties .....  | 2  |
| <b>2</b> | <b>Analysis</b> .....   | 4  |
| <b>3</b> | <b>Production, Processing, Application, Introduction into the Environment</b> ..... | 6  |
| 3.1      | Production .....  | 6  |
| 3.2      | Processing, Application, Consumption Quantities .....                               | 6  |
| 3.3      | Introduction into the Atmosphere .....  | 7  |
| 3.4      | Introduction into the Hydrosphere .....   | 7  |
| 3.5      | Introduction into the Geosphere .....   | 8  |
| 3.6      | Balance of Environmental Introduction .....   | 8  |
| <b>4</b> | <b>Environmental Occurrence</b> .....   | 9  |
| 4.1      | Atmosphere, Geosphere and Hydrosphere .....   | 9  |
| 4.2      | Biota (Animals and Plants) and Food.....  | 9  |
| 4.3      | Other Matrices .....  | 10 |
| <b>5</b> | <b>Environmental Behavior</b> .....   | 12 |
| 5.1      | Biodegradation .....  | 12 |
| 5.2      | Abiotic Degradation .....   | 12 |
| 5.3      | Accumulation .....  | 13 |
| 5.4      | Distribution in the Environmental.....  | 13 |
| 5.5      | Environmental Fate .....  | 15 |

|          |  |    |
|----------|--|----|
| <b>6</b> | <b>Ecotoxicity</b> .....                       | 16 |
| 6.1      | Aquatic Organisms .....                        | 16 |
| 6.1.1    | Microorganisms .....                           | 16 |
| 6.1.2    | Plants .....                                   | 16 |
| 6.1.3    | Invertebrates .....                            | 17 |
| 6.1.4    | Vertebrates .....                              | 17 |
| 6.2      | Terrestrial Organisms .....                    | 17 |
| 6.3      | Ecosystems .....                               | 17 |
| 6.4      | PNEC-Derivation .....                          | 17 |
| <br>     |  |    |
| <b>7</b> | <b>Toxicity in Mammals</b> .....               | 18 |
| 7.1      | General Effects .....                          | 18 |
| 7.2      | Mechanism of Action .....                      | 18 |
| 7.3      | Toxicokinetics .....                           | 18 |
| 7.4      | Acute Toxicity .....                           | 19 |
| 7.5      | Subacute, Subchronic and Chronic Toxicity..... | 20 |
| 7.6      | Skin and Mucous Membrane Tolerance .....       | 20 |
| 7.7      | Sensitization .....                            | 21 |
| 7.8      | Genotoxicity .....                             | 21 |
| 7.9      | Carcinogenicity .....                          | 21 |
| 7.10     | Reproduction Toxicity .....                    | 21 |
| 7.11     | Other Effects .....                            | 22 |
| 7.12     | Experiences in Humans .....                    | 22 |
| <br>     |  |    |
| <b>8</b> | <b>Substance-Specific Regulations</b> .....    | 23 |
| <br>     |  |    |
| <b>9</b> | <b>References</b> .....                        | 25 |