



**German Chemical Society**  
**Gesellschaft Deutscher Chemiker**

GDCh-Advisory Committee  
on Existing Chemicals of  
Environmental Relevance (BUA)

**Isodecanol**

BUA Report 149

(December 1993)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 1996

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edited by the GDCh-Advisory  
Committee on Existing Chemicals  
of Environmental Relevance

Beratergremium für  
Umweltrelevante Altstoffe (BUA)



S. Hirzel

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## Foreword

The German Chemicals Act (Chemikaliengesetz - ChemG) of 1980 stipulates that certain existing chemicals must be reported to the competent authority, if they exhibit properties which indicate that they may be hazardous, either alone or in combination with other substances.

In the summer of 1982, an Advisory Committee on Existing Chemicals of Environmental Relevance (BUA) was set up by the German Chemical Society (Gesellschaft Deutscher Chemiker - GDCh). It brings together representatives from the scientific community, the chemical industry and the governmental authorities. This Advisory Committee is responsible for elaborating appropriate solutions for substances of relevance for health and the environment on the basis of voluntary measures. It selects and examines existing chemicals from the aforementioned angles. The testing and evaluation are based on scientific criteria alone.

It was, therefore, necessary to develop priority setting procedures. In a first phase reports were only prepared for priority chemicals. Within the framework of a first priority setting procedure, chemicals were compiled from several priority lists and 135 chemicals were selected for detailed substance reports.

In a second priority setting procedure the survey of the German Chemical Industry Association (VCI) on all substances with a production volume of more than 10 tons per year was used as a starting list. Since this survey covered 4,600 chemicals, BUA decided to process the corresponding list in several stages. The first stage included approx. 1,050 substances with a production volume of more than 1,000 tons per year.

Detailed reports are drawn up on chemicals suspected of having a hazard potential and abridged reports on those presenting only a minor hazard potential, according to the current state of knowledge.

The detailed BUA reports take in both the published literature and data from industry. If data for the evaluation of the chemicals are not available, additional studies are recommended and the results are published as updates to the reports. The reports serve as a basis for the instigation of administrative measures, when there are indications of risks to health or the environment.

Tübingen, May 1993

Ernst Bayer  
Chairman of the Advisory Committee  
on Existing Chemicals  
of Environmental Relevance

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# **BUA Report on**

## **Summary and conclusions**

### **Ecological aspects**

#### **Manufacture, usage and distribution among environmental compartments (discharge, occurrence)**

Every year since about 1988 12000 t isodecanol have been imported into and around 2000 t exported from the Federal Republic of Germany. When West German production is running at full estimated capacity (1990: 20000 to 30000 t/y), total consumption in the Federal Republic of Germany amounts to 30000 to 40000 t/y.

According to an estimation, most of the isodecanol consumed in the Federal Republic of Germany is converted to plasticizers (about 80 %) and raw materials for detergents, cleaners and stabilizers (about 15 %). Less than 5 % is used directly as fuel additive or as solvent.

Discharge into the environment from production and processing is via wastewater and to a minor extent via waste air.

Discharge into wastewater from production amounts to about 17 t/y. As far as is known, in 1991, approx. 70 t were carried into factory wastewater during processing. It is expected that, given the elimination efficiency of the plant's biological wastewater-treatment plant, a much lower quantity of the compound reaches the main drain. Discharge via waste air from production totalled about 25 kg in all in 1991. As far as is known, processing generates a discharge level to the atmosphere of around 270 kg/y. Nothing is known about discharge that occurs from use of isodecanol. These data account for about half of the isodecanol handled in the Federal Republic of Germany. There are no data about discharge from processing or use for the remaining 50 %.

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Since waste is incinerated, no discharge from this source is expected.

No information is available about the occurrence of isodecanol in the environment.

Judging from the available data, appreciable transfer of the compound from water to air is not expected.

The value of 3.94 for  $\log P_{OW}$  suggests that the compound binds strongly to the organic matter of soil whereas the value of the soil sorption coefficient, calculated from the water solubility, suggests moderate to high potential for soil sorption. Labelling of isodecanol with R 51 (Toxic to aquatic organisms) and R 53 (May cause long-term adverse effects in the aquatic environment) is discussed.

### **Degradability**

In the laboratory, isodecanol is inherently biodegradable in water under aerobic conditions. Nothing is known about degradation under anaerobic conditions or in soils. In view of its structure, hydrolytic degradation is not expected.

The half-life for oxidative photochemical degradation by OH free radicals in the atmosphere has been calculated as ranging from 26 hours to 12 days.

### **Bioaccumulation**

No experimental data pertaining to bioaccumulation are available.

The value of 3.94 for  $\log P_{OW}$  suggests a potential for bioaccumulation.

### **Ecotoxic effects**

In the Short Term Respiration Inhibition Test, a feed concentration of 27.7 mg isodecanol/l inhibited the respiration rate of activated

sludge by 17.9 % within an incubation period of 30 minutes (20 to 25 °C), relative to a readily biodegradable peptone solution.

In the Cell Proliferation Inhibition Test performed on *Pseudomonas putida*, no toxic effect was observed in saturated aqueous solution.

In the Fermentation Tube Test carried out on facultatively anaerobic microorganisms, a toxic threshold (24 h) of between 100 and 1000 mg/l was recorded (water solubility at 20 °C: 0.096 g/l).

The specific rate of oxygen uptake by chemolithotropic, pyrites oxidizing bacteria (*Thiobacillus ferrooxidans*) was reduced by 36 % in 90 minutes by 80.46 mg isodecanol/l.

In a Cell Proliferation Inhibition Test performed on the green alga *Scenedesmus subspicatus*, 72-h exposure yielded an EC<sub>10</sub> value of 9.5 mg/l, an EC<sub>50</sub> value of 19 mg/l and an EC<sub>90</sub> value of 40 mg/l.

In a test involving artificial sea water, the 24-h LC<sub>50</sub> value was 3.4 mg/l for the brine shrimp *Artemia salina*. For the marine shrimp *Nitocra spinipes*, a 96-h LC<sub>50</sub> value of 13 mg/l was determined.

No information is available about the effect of isodecanol on *Daphnia* or fish.

### **Toxicological aspects**

The metabolism of fatty alcohol mixtures consists in oxidation to the corresponding fatty acid via paths in the lipometabolism.

Isodecanol is only slightly toxic but irritates the skin and severely irritates the eyes.

In the Ames Test, both with and without metabolic activation, isodecanol is not mutagenic. Isodecanol is not clastogenic in mammalian cells (V 79), whether with or without metabolic activation.

## XIV

Fourteen days' oral administration of 168 mg/kg isodecanol did not produce signs in rats of peroxisome proliferation, testicular atrophy, hepatomegaly or hypolipidaemia. A concentration of 1580 mg/kg proved lethal to pregnant Wistar rats and, in the surviving animals, primarily produced symptoms of an hepatotoxic effect. A subchronic study that satisfies today's standards does not exist.

Embryotoxic/teratogenic effects were only observed at the maternal toxicity level.

No information is available about sensitization, chronic toxicity or carcinogenicity.

No experience has been gained of its effects on humans.

### **Recommendations**

#### **Ecological aspects**

As there are no data about discharge from processing or use for 50 % of the isodecanol consumption in the Federal Republic of Germany, discharge from use in Germany should be cleared up.

In view of the lack of information on toxicity to fish, a 96-h fish test should be performed on the zebra fish *Brachydanio rerio*.

#### **Toxicological aspects**

Studies of carcinogenicity and sensitization are, especially for structural reasons, in the light of current knowledge not considered urgent.