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Ethylbenzene in Drinking-water

Background document for development of
WHO *Guidelines for Drinking-water Quality*

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Preface

One of the primary goals of WHO and its member states is that "all people, whatever their stage of development and their social and economic conditions, have the right to have access to an adequate supply of safe drinking water." A major WHO function to achieve such goals is the responsibility "to propose regulations, and to make recommendations with respect to international health matters ...."

The first WHO document dealing specifically with public drinking-water quality was published in 1958 as International Standards for Drinking-Water. It was subsequently revised in 1963 and in 1971 under the same title. In 1984–1985, the first edition of the WHO Guidelines for drinking-water quality (GDWQ) was published in three volumes: Volume 1, Recommendations; Volume 2, Health criteria and other supporting information; and Volume 3, Surveillance and control of community supplies. Second editions of these volumes were published in 1993, 1996 and 1997, respectively. Addenda to Volumes 1 and 2 of the second edition were published in 1998, addressing selected chemicals. An addendum on microbiological aspects reviewing selected microorganisms was published in 2002.

The GDWQ are subject to a rolling revision process. Through this process, microbial, chemical and radiological aspects of drinking-water are subject to periodic review, and documentation related to aspects of protection and control of public drinking-water quality is accordingly prepared/updated.

Since the first edition of the GDWQ, WHO has published information on health criteria and other supporting information to the GDWQ, describing the approaches used in deriving guideline values and presenting critical reviews and evaluations of the effects on human health of the substances or contaminants examined in drinking-water.

For each chemical contaminant or substance considered, a lead institution prepared a health criteria document evaluating the risks for human health from exposure to the particular chemical in drinking-water. Institutions from Canada, Denmark, Finland, France, Germany, Italy, Japan, Netherlands, Norway, Poland, Sweden, United Kingdom and United States of America prepared the requested health criteria documents.

Under the responsibility of the coordinators for a group of chemicals considered in the guidelines, the draft health criteria documents were submitted to a number of scientific institutions and selected experts for peer review. Comments were taken into consideration by the coordinators and authors before the documents were submitted for final evaluation by the experts meetings. A "final task force" meeting reviewed the health risk assessments and public and peer review comments and, where appropriate, decided upon guideline values. During preparation of the third edition of the GDWQ, it was decided to include a public review via the world wide web in the process of development of the health criteria documents.

During the preparation of health criteria documents and at experts meetings, careful consideration was given to information available in previous risk assessments carried out by the International Programme on Chemical Safety, in its Environmental Health

Criteria monographs and Concise International Chemical Assessment Documents, the International Agency for Research on Cancer, the joint FAO/WHO Meetings on Pesticide Residues, and the joint FAO/WHO Expert Committee on Food Additives (which evaluates contaminants such as lead, cadmium, nitrate and nitrite in addition to food additives).

Further up-to-date information on the GDWQ and the process of their development is available on the WHO internet site and in the current edition of the GDWQ.

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GENERAL DESCRIPTION

Identity

CAS no.: 100-41-4
Molecular formula: C_8H_{10}

Physical and chemical properties (*1*) [Conversion factor in air: 1 ppm = 4.35 mg/m^3]

Property	*Value*
Physical state	Colourless liquid
Melting point	-95 °C
Boiling point	136.2 °C
Vapour pressure	0.933 kPa at 20 °C
Density	0.86 g/cm^3 at 20 °C
Water solubility	152 mg/litre at 20 °C
Log octanol–water partition coefficient	3.15

Organoleptic properties

Ethylbenzene has an aromatic odour. The odour threshold is in the range 0.27–0.4 mg/m^3 in air (*1,2*) and 0.002–0.13 mg/litre in water (*1,3*). The taste threshold ranges from 0.072 to 0.2 mg/litre (*2,3*).

Major uses

Ethylbenzene is present in xylene mixtures at levels up to 15–20% (*4*). This mixture is used in the paint industry, in insecticide sprays, and in petrol blends. Ethylbenzene is used primarily in the production of styrene and acetophenone, as a solvent, and as a constituent of asphalt and naphtha.

Environmental fate

The primary source of ethylbenzene in the environment is the petroleum industry. Because of its high vapour pressure and low solubility, it will disperse into the atmosphere if released. More than 96% of ethylbenzene can be expected in the air compartment. It is phototransformed in the air by reaction with hydroxyl radicals; the half-life is approximately 1 day (*5*).
Biodegradation of ethylbenzene in soil under aerobic conditions with a half-life of 24.2 days has been reported. In activated sludge and water, it can be biodegraded under aerobic conditions (*6*).

ANALYTICAL METHODS

A purge-and-trap gas chromatographic procedure with photoionization detection can be used for the determination of ethylbenzene in water over a concentration range of 0.02–1500 µg/litre (*7*). Confirmation is by mass spectrometry (*8*). Methods for the determination of ethylbenzene in air, soil, and other matrices have been reviewed and compiled by Fishbein & O'Neill (*9*). Continuous monitoring of ethylbenzene and other volatile hydrocarbons is possible at the microgram per litre level (*10*).

ENVIRONMENTAL LEVELS AND HUMAN EXPOSURE

Air

In Germany, average indoor and outdoor ethylbenzene concentrations of 13 μg/m^3 were found (*11*). In Italy, mean indoor and outdoor air concentrations of 27 and 7.4 μg/m^3 were reported (*12*).
The median daily concentrations of ethylbenzene in the urban air of nine major cities in the USA of 1.3–6.5 μg/m^3 (*13*). In the Netherlands, mean and maximum values of 0.9–2.8 and 10.0–25.7 μg/m^3, respectively, were reported (*14*).

Water

The maximum ethylbenzene concentration in the Besós river in Spain was 15 μg/litre and in the Llobregat river 1.9 μg/litre (*15*). Levels of 0.03–0.3 mg/litre were reported in groundwater contaminated by point emissions (*16*).

In a survey of groundwater supplies (*17*), it was found that approximately 0.6% of 945 such supplies contained ethylbenzene; the median concentration was 0.87 μg/litre. In the Netherlands, ethylbenzene was detected in 1% of 304 samples of groundwater (*18*); the maximum concentration was 0.4 μg/litre. Concentrations of up to 0.07 μg/litre were found in aquifers in the United Kingdom (*19*). In Canada, in a study of 30 water-treatment plants, concentrations in drinking-water were below 1 μg/litre (*20*).

In Los Angeles, USA, an ethylbenzene concentration of 9 ng/litre was found in rainwater (*21*).

Food

Ethylbenzene has been identified in volatiles of roasted hazelnuts. It can migrate from polystyrene food packaging into food. Concentrations of 2.5–21 μg/litre have been reported in milk and soup (*5*).

Estimated total exposure and relative contribution of drinking-water

Although there is little information concerning the intake of ethylbenzene via food and drinking-water, it is expected to be low compared with that via air. In the Netherlands, the estimated daily exposure is 40 μg (*14*), based on a ventilation volume of 20 m^3/day.

KINETICS AND METABOLISM IN LABORATORY ANIMALS AND HUMANS

Ethylbenzene in liquid form is easily absorbed by humans via both the skin and the intestinal tract (exact absorption percentages not reported); the vapour is readily absorbed when inhaled (reported absorption percentage 64% for humans, 44% for rats). Both distribution and excretion are rapid. In humans, storage of ethylbenzene in fat has been reported, and the compound has been observed to pass the placental barrier. Biotransformation in humans is almost completely to mandelic acid and phenylglyoxalic acid, both these metabolites being excreted in urine. Metabolism in experimental animals differs from that in humans in that benzoic acid is the major metabolite together with mandelic acid. Urinary excretion of metabolites is almost complete within 24 h (*1,5*).

EFFECTS ON LABORATORY ANIMALS AND *IN VITRO* TEST SYSTEMS

Acute exposure

Ethylbenzene has a low acute toxicity via the oral route; LD_{50}s in rats range from 3.5 to 4.7 g/kg of body weight (*22*).

Short-term exposure

In a short-term oral study in rats, effects on liver and kidneys were observed at 400 mg/kg of body weight and higher dose levels (administered 5 days per week for 6 months); there were no such effects at 136 mg/kg of body weight (*23*). Liver effects were also found in a number of inhalation studies; the LOAEL for this type of effect was 1305 mg/m^3, no effects being seen at 218 or 430 mg/m^3 (concentrations administered for 6 h per day, 5 days per week) (*5,24,25*).

Reproductive toxicity, embryotoxicity, and teratogenicity

In all the teratogenicity studies in rats and rabbits, dosing was via the inhalation route. No definite conclusions with regard to the observed effects (maternal toxicity, reduced fertility and, possibly, teratogenicity) can be drawn from the reports available (*5,22*).

Mutagenicity and related end-points

Studies were carried out in bacteria, yeasts, insects, mammalian cells (*in vitro*), and intact mammals; negative results were obtained in all test systems, showing ethylbenzene to be devoid of mutagenic activity (*1,5,22*).

EFFECTS ON HUMANS

Relevant oral data are lacking. Data for the inhalation route are limited to acute studies considered insufficient as a basis for a guideline value (*1,5,22*).

GUIDELINE VALUE

No carcinogenicity data on ethylbenzene are available. The compound was shown to be nonmutagenic in a number of tests. Given these findings, a TDI approach may be applied. The TDI is derived using a NOAEL of 136 mg/kg of body weight per day based on hepatotoxicity and nephrotoxicity observed in a limited 6-month study in rats (administration 5 days per week) (*23*); this dose level is equivalent to 97.1 mg/kg of body weight per day for dosing 7 days per week. After application of an uncertainty factor of 1000 (100 for intra- and interspecies variation and 10 for the limited database and short duration of the study), a TDI of 97.1 µg/kg of body weight results. This yields a guideline value of 300 µg/litre (rounded figure), allocating 10% of the TDI to drinking-water, which exceeds the lowest reported odour threshold in drinking-water (2.4 µg/litre).

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