EUROPEAN COMMISSION
Institute for Health and Consumer Protection
Toxicology and Chemical Substance (TCS)
European Chemicals Bureau
I-21020 Ispra (VA) Italy

NITROBENZENE

Part I – Environment

CAS No: 98-95-3

EINECS No: 202-716-0

Summary Risk Assessment Report

2008 **EUR 22480 EN/2**

The mission of the IHCP is to provide scientific support to the development and implementation of EU polices related to health and consumer protection. The IHCP carries out research to improve the understanding of potential health risks posed by chemical, physical and biological agents from various sources to which consumers are exposed.

The Toxicology and Chemical Substances Unit (TCS), commonly known as the European Chemicals Bureau (ECB), provides scientific and technical input and know-how to the conception, development, implementation and monitoring of EU policies on dangerous chemicals including the co-ordination of EU Risk Assessments. The aim of the legislative activity of the ECB is to ensure a high level of protection for workers, consumers and the environment against dangerous chemicals and to ensure the efficient functioning of the internal market on chemicals under the current Community legislation. It plays a major role in the implementation of REACH through development of technical guidance for industry and new chemicals agency and tools for chemical dossier registration (IUCLID5). The TCS Unit ensures the development of methodologies and software tools to support a systematic and harmonised assessment of chemicals addressed in a number of European directives and regulation on chemicals. The research and support activities of the TCS are executed in close co-operation with the relevant authorities of the EU Member States, Commission services (such as DG Environment and DG Enterprise), the chemical industry, the OECD and other international organisations.

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SUMMARY RISK ASSESSMENT REPORT

Final report, 2008

Germany

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Date of Last Literature Search:	**1998**
Review of report by MS Technical Experts finalised:	**April 2005**
Final report:	**2008**

PREFACE

This report provides a summary, with conclusions, of the risk assessment report of the substance nitrobenzene that has been prepared by Germany in the context of Council Regulation (EEC) No. 793/93 on the evaluation and control of existing substances.

For detailed information on the risk assessment principles and procedures followed, the underlying data and the literature references the reader is referred to the comprehensive Final Risk Assessment Report (Final RAR) that can be obtained from the European Chemicals Bureau[1]. The Final RAR should be used for citation purposes rather than this present Summary Report.

[1] European Chemicals Bureau – Existing Chemicals – http://ecb.jrc.it

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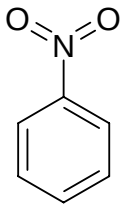
1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

CAS No: 98-95-3
EINECS No: 202-716-0
IUPAC Name: nitrobenzene
Synonyms: Nitrobenzol, Benzene, Nitro-, Essence of Mirbane; Essence of Myrbane, Mirbane Oil; Myrbane Oil, Mononitrobenzene
Molecular formula: $C_6 H_5 N O_2$
Molecular weight:: 123 g/mol
Structural formula:



1.2 PURITY/IMPURITIES, ADDITIVES

Purity: > 98.9%

Impurities: Benzene
o-Nitrotoluene
p-Nitrotoluene
p-Dinitrobenzene
m-Dintirobenzene
o-Dinitrobenzene
Toluene
Water

1.3 PHYSICO-CHEMICAL PROPERTIES

Table 1.1 Summary of physico-chemical properties

Property	Value
Physical state	liquid
Melting point	5.26°C
Boiling point	210.8°C
Relative density	1.2037
Vapour pressure	0.2 hPa at 20°C 32.6 Pa at 25°C
Water solubility	1,900 mg/l at 20°C
Partition coefficient n-octanol/water (log value)	1.86 at 24.5°C
Flash point	88°C
Autoflammability	480°C (DIN 51794)
Flammability	Not extremely flammable Not highly flammable Not flammable
Explosive properties	No explosive properties
Oxidizing properties	Not applicable (liquid)
Henry's constant	1.296 $Pa \cdot m^3 \cdot mol^{-1}$ at 20°C 2.16 $Pa \cdot m^3 \cdot mol^{-1}$ at 25°C [5)]
Surface tension	43.9 mN/m at 20°C (pure substance)

1.4 CLASSIFICATION

1.4.1 Current classification

For the environment nitrobenzene is classified with N; R51-53 (had been included in the 22nd ATP).

The current classification is T, N; R 23/24/25-48/23/24-40-62-51/53.

1.4.2 Proposed classification

The data presented in the Risk Assessment Report do not support the current classification as N; R51-53. According to this data the current classification should be changed from N; R51-53 to N; R52-53.

2 GENERAL INFORMATION ON EXPOSURE

There is no natural source of nitrobenzene known. Nitrobenzene is almost exclusively produced by nitration of benzene. Nitrobenzene is mainly used as an intermediate in the manufacture of aniline.

According to available data there are 8 production and/or processing sites of nitrobenzene within the EU. There are no imports or exports of nitrobenzene known. The resultant quantity of nitrobenzene marketed in the EU amounts to be $1.18 \cdot 10^6$ tonnes/year.

Almost all nitrobenzene is used for the production of aniline (99%) and, to a much lesser extent, for the production of pharmaceuticals (0.8%) and various other chemicals (0.2%).

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

Releases of nitrobenzene into the environment are to be expected during production and processing to waste water and, to a lesser extend, exhaust gases. Further emissions to air are expected from waste water treatment plants. Direct releases to agricultural or natural soil are not expected.

According to Mackay model (level 1) the hydrosphere is the target compartment for nitrobenzene (68.5%), followed by the atmosphere (30.7%).

Nitrobenzene is not expected to hydrolyse under environmental conditions. Photodegradation (i.e. direct photolysis and photooxidation) in air and water does not play an important role either. Nitrobenzene is considered to be not inherently biodegradable. However, measured removal rates by adapted microorganisms are > 90% in industrial STP. The mean value of 92.8% was used for all production and processing sites.

The calculated K_{oc} value of 118 l/kg (based on log K_{ow} of 1.86) does not indicate a significant adsorption potential. If nitrobenzene is released or deposited to soil most of the substance is expected to leach through the soil into the groundwater.

The calculated Henry´s law constant of 1.296 $Pa \cdot m^3 \cdot mol^{-1}$ indicates medium volatility from surface water. The potential for bioaccumulation is low.

Predicted Environmental Concentrations (PEC) (sum of local and regional concentration; $PEC_{regional}$ = 0.01 µg/l) are calculated for the local aquatic environments of the production and processing sites using all site-specific information available. If no site-specific information was available, the default values from the TGD were used. The resulting PEClocal range between 0.03 µg/l and 8.35 µg/l (production and processing), and between 0.01 µg/l and 0.02 µg/l (processing only). Most of the 90-percentile values measured in surface water are below 1 µg/l.

The PEC for microorganisms in the STP (PEC_{stp}) equals the concentration in the effluent of a STP. The concentrations in the specific STPs vary from < 1 µg/l to 140 µg/l. However, a much higher PEC_{stp} of 1,000 µg/l occurs at one site (reed bed system).

As nitrobenzene is not expected to adsorb to organic matter, $PEC_{sediment}$ is calculated based on highest PEC_{local} for water. A $PEC_{sediment}$ = 0.03 mg/kg_{ww} results.

Nitrobenzene is expected to enter the soil as a result of deposition from the atmosphere. The input through sludge application on agricultural soil is considered negligible. Considering this route of exposure, the highest local concentration in soil can be expected as 2.3 $\mu g/kg_{ww}$ (production and processing) using a $PEC_{regional}$ of 5.4 ng/kg_{ww}. The given local PEC_{soil} corresponds to a $PEC_{soil\text{-}porewater}$ of 1.1 µg/l.

For the exposure calculation for the atmosphere, site-specific data are used as far as they were submitted. $PEC_{localair}$ between 0.021 and 0.46 $\mu g/m^3$ ($PEC_{regional}$ = 0.05 ng/m^3) were calculated.

3.2 EFFECTS ASSESSMENT: HAZARD IDENTIFICATION AND DOSE (CONCENTRATION) - RESPONSE (EFFECT ASSESSMENT)

3.2.1 Aquatic compartment (incl. sediment)

Results from acute toxicity tests with species from 3 trophic levels are available. The most sensitive organisms from standard tests (EC_{50}) are *Oryzias latipes, Daphnia magna* and *Chlorella pyrenoidosa.*

Reliable long-term NOECs are available for invertebrates (*Daphnia magna*) and several algae species. The most sensitive value has been determined for *Daphnia magna* with a 21-day NOEC of 1.9 mg/l. This leads to a $PNEC_{aqua}$ of 38 µg/l applying an assessment factor of 50.

Different tests with microorganisms, bacteria and protozoa are available for the determination of the $PNEC_{stp}$.

The lowest effect concentration found was for *Nitrosomonas* with a 24-hour IC_{50} of 0.92 mg/l. Applying an assessment factor of 10 leads to a $PNEC_{stp}$ = 92 µg/l. This PNEC is used for the risk characterisation of STP at all sites except site E.

For the assessment of the reed bed system at site E the activated sludge respiration inhibition test was considered. It leads to a 3-hour EC_{50} of 100 mg/l. Applying an assessment factor of 100 results in a $PNEC_{stp}$ of 1 mg/l for the assessment of this specific site.

As there is a lack of tests on sediment-dwelling organisms the equilibrium partitioning method was used to calculate the $PNEC_{sediment}$ of 0.127 mg/kg_{ww}.

3.2.2 Terrestrial compartment

There is only one terrestrial test result available (earthworm) for the calculation of the PNE_{soil}. It is calculated with the most sensitive of the earthworm species *Eudrilus eugeniae* with a 14-day LC_{50} of 226 mg/kg $soil_{dw}$ and an assessment factor of 1,000. A $PNEC_{soil}$ = 0.226 mg/kg_{dw} can be derived.

As there is only one terrestrial test result available the TGD instructs that the risk assessment should be performed both on this test result and on the basis of the outcome of the aquatic toxicity data in this case. A $PNEC_{soil}$ of 0.10 mg/kg_{dw} can be derived by using the equilibrium partitioning method.

The use of the equilibrium partitioning method based on the $PNEC_{water}$ results in a lower $PNEC_{soil}$. Thus, the $PNEC_{soil}$ of 0.10 mg/ kg_{dw} (0.084 mg/kg_{ww}) derived from the equilibrium partitioning is used for risk assessment.

3.2.3 Atmosphere

There are no representative fumigation tests for nitrobenzene available. The only result is a 3-hour LOEC (photosynthetic rate) of 150 mg/m^3 *(Triticum aestivum).*

3.2.4 Secondary poisoning

Secondary poisoning is considered not to be relevant for nitrobenzene.

3.3 RISK CHARACTERISATION [2]

The PEC/PNEC ratios for surface water are below 1 for all production and/or processing sites. **Conclusion (ii)**.

The highest PEC/PNEC ratio for sediment is the same as for water as both the PEC and the PNEC are calculated from the respective water values. Hence no risk for sediment dwelling organisms can be detected. **Conclusion (ii)**.

Applying the $PNEC_{microorganisms}$ of 92 µg/l for the industrial STP at all sites except for site E and the $PNEC_{microorganisms}$ of 1000 µg/l for the constructed wetland at site E all ratios of $PEC/PNEC_{microorganisms}$ are ≤ 1. **Conclusion (ii)**.

The comparison of $PEClocal_{soil}$ of $2.3 \cdot 10^{-3}$ mg/kg_{ww} with the $PNEC_{soil}$ of 0.084 mg/kg_{ww} indicates no risk for the terrestrial compartment. **Conclusion (ii)**.

There are no representative fumigation tests for nitrobenzene available. A quantitative effect assessment for the atmosphere can therefore not be performed. The only result is a 3-hour LOEC of 150 mg/m^3. Comparing this result with the highest $PEClocal_{air\_annual}$ of $4.6 \cdot 10^{-4}$ mg/m^3 no risk to terrestrial plants via air emissions of nitrobenzene can be found as the ratio of $PEClocal_{air\_annual}$ /LOEC is very small ($3 \cdot 10^{-6}$). In a first approach nitrobenzene does not pose a risk to plants. **Conclusion (ii)**.

As nitrobenzene has only a low bioaccumulation potential no risk characterisation for secondary poisoning was conducted. Nitrobenzene does not meet the PBT criteria.

[2] Conclusion (i) There is a need for further information and/or testing.
Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.
Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

4 HUMAN HEALTH

(to be added later)

5 RESULTS

5.1 ENVIRONMENT

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (ii) applies to surface water, sediment, the atmosphere and the terrestrial compartment regarded for the production and/or processing of nitrobenzene. All PEC/PNEC ratios are below 1. This conclusion also applies to the industrial STP of all sites.

European Commission

EUR 22480 EN/2 **Summary Risk Assessment Report**
Nitrobenzene, part I - environment

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The report provides the summary of the comprehensive risk assessment of environment part of the substance nitrobenzene. It has been prepared by Germany in the frame of Council Regulation (EEC) No. 793/93 on the evaluation and control of the risks of existing substances, following the principles for assessment of the risks to humans and the environment, laid down in Commission Regulation (EC) No. 1488/94.

Part I – Environment

The evaluation considers the emissions and the resulting exposure to the environment in all life cycle steps. Following the exposure assessment, the environmental risk characterisation for each protection goal in the aquatic, terrestrial and atmospheric compartment has been determined.

The environmental risk assessment for nitrobenzene concludes that risks are not expected.

Part II – Human Health

This part of the evaluation will be published later.