European Union Risk Assessment Report

European Chemicals Bureau

Existing Substances

propan-1-ol
part I - environment

CAS No: 71-23-8  EINECS No: 200-746-9

propan-1-ol

H_3C

CH_2

CH_2

OH

2nd Priority List

Volume: 82
The mission of the IHCP is to provide scientific support to the development and implementation of EU policies 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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European Union Risk Assessment Report

PROPAN-1-OL

Part I – environment

CAS-No: 71-23-8
EINECS-No: 200-746-9

RISK ASSESSMENT
The first draft of the Comprehensive Risk Assessment Report of propan-1-ol, a substance chosen from the EU 2nd priority list in 1995 was distributed for the preliminary written procedure in June 2002.

The “in depth discussion” was at the Technical Meeting in March 2003 (TM I’03).

This document is a revised draft of the environmental part of the Risk Assessment Report which is intended to be discussed as “final written approval” at the Technical Meeting in September 2003 (TM III’03).

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Date of Last Literature Search: 2001
Review of report by MS Technical Experts finalised: August 2003
Final report: 2008
Foreword

We are pleased to present this Risk Assessment Report which is the result of in-depth work carried out by experts in one Member State, working in co-operation with their counterparts in the other Member States, the Commission Services, Industry and public interest groups. The Risk Assessment was carried out in accordance with Council Regulation (EEC) 793/93\(^1\) on the evaluation and control of the risks of "existing" substances. "Existing" substances are chemical substances in use within the European Community before September 1981 and listed in the European Inventory of Existing Commercial Chemical Substances. Regulation 793/93 provides a systematic framework for the evaluation of the risks to human health and the environment of these substances if they are produced or imported into the Community in volumes above 10 tonnes per year.

There are four overall stages in the Regulation for reducing the risks: data collection, priority setting, risk assessment and risk reduction. Data provided by Industry are used by Member States and the Commission services to determine the priority of the substances which need to be assessed. For each substance on a priority list, a Member State volunteers to act as "Rapporteur", undertaking the in-depth Risk Assessment and recommending a strategy to limit the risks of exposure to the substance, if necessary.

The methods for carrying out an in-depth Risk Assessment at Community level are laid down in Commission Regulation (EC) 1488/94\(^2\), which is supported by a technical guidance document\(^3\). Normally, the "Rapporteur" and individual companies producing, importing and/or using the chemicals work closely together to develop a draft Risk Assessment Report, which is then presented at a meeting of Member State technical experts for endorsement. The Risk Assessment Report is then peer-reviewed by the Scientific Committee on Health and Environmental Risks (SCHER) which gives its opinion to the European Commission on the quality of the risk assessment.

If a Risk Assessment Report concludes that measures to reduce the risks of exposure to the substances are needed, beyond any measures which may already be in place, the next step in the process is for the "Rapporteur" to develop a proposal for a strategy to limit those risks. The Risk Assessment Report is also presented to the Organisation for Economic Co-operation and Development as a contribution to the Chapter 19, Agenda 21 goals for evaluating chemicals, agreed at the United Nations Conference on Environment and Development, held in Rio de Janeiro in 1992 and confirmed in the Johannesburg Declaration on Sustainable Development at the World Summit on Sustainable Development, held in Johannesburg, South Africa in 2002. This Risk Assessment improves our knowledge about the risks to human health and the environment from exposure to chemicals. We hope you will agree that the results of this in-depth study and intensive co-operation will make a worthwhile contribution to the Community objective of reducing the overall risks from exposure to chemicals.

Roland Schenkel
Director General
DG Joint Research Centre

Mogens Peter Carl
Director General
DG Environment

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\(^1\) O.J. No L 084, 05/04/1999 p.0001 - 0075

\(^2\) O.J. No L 161, 29/06/1994 p. 0003 - 0011

OVERALL RESULTS OF THE RISK ASSESSMENT

CAS No: 71-23-8  
EINECS No: 200-746-9  
IUPAC Name: propan-1-ol

Overall results of the risk assessment:

Conclusion (i) There is 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.

Summary of conclusions:

Environment

From the intrinsic properties it is expected that propan-1-ol is of low concern for the environment. The environmental risk assessment was performed, using conservative estimates based on worst-case assumptions at the exposure and effects side. The risk assessment results in the following conclusion:

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.

Based on the currently available data, propan-1-ol represents no risk to the environment for the area of production, processing, formulation and use.

Human Health

Workers

Conclusion (i) There is need for further information and/or testing.

For mutagenicity the base set data have to be completed, risk assessment concerning carcinogenicity will be delayed until the mutagenicity data are available.

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

Summary of conclusions:

There is a need for limiting the risks of propan-1-ol for several scenarios with short-term and repeated exposures. The most critical exposure route is inhalation, dermal contact being of minor importance. In detail concern is expressed for use of paints, use of cleaning formulations without LEV, short term exposures during use of printing inks.

The toxic effects leading to concern are respiratory depression according to stimulation of the trigeminus nerve, local effects in the airways after repeated exposure and reproductive toxicity concerning fertility as well as developmental toxicity. Risk reduction measures especially for the inhalative exposure situation have to be initiated.
Consumers

Conclusion (i) There is need for further information and/or testing.

Mutagenicity

The minimum requirements in mutagenic testing are not met. An *in vitro* study on chromosome aberration in Chinese hamster cells is currently ongoing.

The producer has to be requested to make available existing studies.

Carcinogenicity

There is no valid carcinogenicity study available. The present data base gives no indication for carcinogenic effects. For performing the risk assessment on carcinogenicity, however, the completed data on mutagenicity have to be taken into account.

Humans exposed indirectly via the 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.
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1.3 CLASSIFICATION

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1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS No:</td>
<td>71-23-8</td>
</tr>
<tr>
<td>EINECS No:</td>
<td>200-746-9</td>
</tr>
<tr>
<td>IUPAC Name:</td>
<td>Propan-1-ol</td>
</tr>
<tr>
<td>Synonyms:</td>
<td>1-hydroxypropane, 1-propanol, ethylcarbinol, n-propanol, n-propyl alcohol, propanol-1, alcohol C3</td>
</tr>
<tr>
<td>Empirical formula:</td>
<td>C₃H₈O</td>
</tr>
<tr>
<td>Molecular weight:</td>
<td>60.1 g/mol</td>
</tr>
<tr>
<td>Structural formula:</td>
<td><img src="attachment" alt="Structural formula" /></td>
</tr>
</tbody>
</table>

1.2 PURITY/IMPURITIES, ADDITIVES

- **Purity:** > 99%
- **Impurities:**
  - methanol
  - ethanol
  - C6 aldehydes
  - propyl propionate
  - 2-methylvaleraldehyde
  - ≤ 0.2% w/w aldehyde
  - < 0.1 w/w dipropyl ether
  - ≤ 0.1% w/w water
  - ≤ 0.003% w/w acetic acid
Table 1.1 Physico-chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Result</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>clear colourless liquid with characteristic odour</td>
<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>-126.5°C</td>
<td>CRC Handbook (1991/92)</td>
</tr>
<tr>
<td>Boiling point</td>
<td>97.1°C at 1,013 hPa</td>
<td>Hiaki et al. (1994)</td>
</tr>
<tr>
<td>Density</td>
<td>0.803 g/cm³ at 20°C</td>
<td>Wilhoit and Zwolinski (1973)</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>19.4 hPa at 20°C</td>
<td>Hiaki et al. (1994)</td>
</tr>
<tr>
<td>Surface tension</td>
<td>67.1 mN/m at 25°C c=1 g/l</td>
<td>CRC Handbook (1991/92)</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>0.34 (shake flask method)</td>
<td>Hansch and Anderson (1967)</td>
</tr>
<tr>
<td>Water solubility</td>
<td>completely soluble</td>
<td>Yaws et al. (1990)</td>
</tr>
<tr>
<td>Flash point</td>
<td>22°C (corrected to the presence of iso-propanol) 23.5°C (99.9% pure)</td>
<td>CHEMSAFE</td>
</tr>
<tr>
<td>Auto flammability</td>
<td>385°C</td>
<td>CHEMSAFE</td>
</tr>
<tr>
<td>Flammability</td>
<td>flammable</td>
<td>CHEMSAFE</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>not explosive</td>
<td>due to structural reasons</td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>no oxidising properties</td>
<td>due to structural reasons</td>
</tr>
</tbody>
</table>

Vapour pressure

The values given for the vapour pressure at 20°C vary between 19 and 20.3 hPa. In the safety data sheet of the BASF AG a value of 19.4°C is quoted, in the data sheet of the Hoechst AG the vapour pressure is quoted with 20 hPa. In both cases no other information is given. Also without any further information Sasol has quoted a value of 20 hPa at 20°C. For the risk assessment the value of 19.4 hPa at 20°C is recommended. This value is derived from the Antoine equation determined by Boublik T, Fried V and Hala E (1984).

Partition coefficient n-octanol/water

The values for the partition coefficient n-octanol/water are varying between 0.25 and 0.38. The safety data sheets of the BASF AG, Hoechst AG and Union Carbide are quoting values between 0.25 and 0.34 without further information. Furthermore the partition coefficients are calculated. The following values are found: 0.271 (according to Rekker with program PRO-LOGP, ver.2 from CompuDrug Ltd.), 0.38 (Abraham MH, Chadha HS, Whiting GS and Mitchell RC (1994)). Further undocumented values are quoted by Petrasol BV, Gorinchem and BASF AG (1989): Labor fuer Umweltanalytik by 0.25 and 0.271, respectively. Other values from literature are in the above mentioned range.

For risk assessment the value of 0.34 of Hansch C and Anderson SM is recommended. The authors have great experience in the field of measuring and calculating octanol/water partition coefficients. They used some kind of shake flask method (Hansch C and Anderson SM (1967)).
Flash point

The value of 23.5°C was determined for n-propanol with a purity of 99.9%. The tests were conducted according to DIN 51755 (Testing of mineral oils and other combustible liquids; determination of flash point by the closed tester according to Abel-Pensky) and ISO 3679 (Paints, varnishes, petroleum and related products - determination of flashpoint – rapid equilibrium method). The value of 23.5°C was corrected for commercial n-propanol to 22°C because of iso-propanol which is usually present as an impurity.

1.3 CLASSIFICATION

- (Classification according to Annex I)4

<table>
<thead>
<tr>
<th>Category</th>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highly flammable</td>
<td>R 11</td>
<td>Highly flammable</td>
</tr>
<tr>
<td>Irritant</td>
<td>R 41</td>
<td>Risk of serious damage to eyes</td>
</tr>
<tr>
<td></td>
<td>R 67</td>
<td>Vapours may cause drowsiness and dizziness</td>
</tr>
</tbody>
</table>

- (Proposal of the rapporteur)

<table>
<thead>
<tr>
<th>Category</th>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flammable</td>
<td>R 10</td>
<td>Flammable</td>
</tr>
<tr>
<td>Irritant</td>
<td>R 41</td>
<td>Risk of serious damage to eyes</td>
</tr>
</tbody>
</table>

A value of 23.5°C was determined for the flash point of n-propanol with a purity of 99.9%. This value of 23.5°C was corrected for commercial n-propanol which usually contains iso-propanol as an impurity to 22°C.

The classification for liquid substances with a flash point between 21 and 55°C is “flammable”.

Therefore the legal classification according to Annex I for propan-1-ol which is at the moment “highly flammable” must be corrected. The original classification resulted from measurements of n-propanol contaminated with impurities (flash point < 21°C).

According to the data presented below and the criteria of Directive 93/21/EEC propan-1-ol has not to be classified as dangerous for the environment.

Propan-1-ol is classified according to water-hazard class 1 (slightly hazardous to water).

---

2 GENERAL INFORMATION ON EXPOSURE

2.1 PRODUCTION

According to the information from the currently available IUCLID data sets there is one production site of propan-1-ol in the EU. The chemical is imported by 5 other companies from outside of the EU. There is no information on possible exports of propan-1-ol.

Based on the production and import quantities approximately 30,100 tonnes/annum of propan-1-ol are used in the EU.

Propan-1-ol is produced almost exclusively by the reaction of ethene with synthesis gas. Reaction is performed at 25-30 MPa and 140-180°C in the liquid phase in the presence of cobalt carbonyl hydrogen as catalyst. After the separation of the catalyst the raw mixture obtained can be hydrogenated in the gaseous phase on the nickel catalyst (0.2-0.3 MPa, 115°C) or on the copper catalyst (3-5 MPa, 130-160°C) and in the liquid phase (8 MPa, 115°C) on the nickel catalyst. By means of subsequent distillation the production of pure propan-1-ol is achieved (Weissermel and Arpe, 1988; Falbe et al., 1980).

2.2 PROCESSING/APPLICATION (CATEGORIES OF USE, AMOUNTS)

In Western Europe propan-1-ol is mainly used as solvent for the formulation of disinfectants, pharmaceutical products, cleaning agents, paints, coating materials, enamel and lacquer paints, printing inks and cosmetics (GDCh, 1997).

Propan-1-ol is processed chemically to intermediates such as propylamines, carboxylic acid esters and halogenated hydrocarbons, which in turn are needed for the synthesis of herbicides, aroma and perfume substances, cosmetics and pharmaceuticals (GDCh, 1997).

Of the propan-1-ol produced by BASF AG, 10% were processed to intermediates and 90% were used as solvent; application areas as solvent were paints, surface coatings and inks, cosmetics and pharmaceuticals, detergents and other (BASF, 1994).

Hoechst AG manufactured 5,000 tonnes of propan-1-ol in 1993; about 3,500 tonnes were processed to n-propylamines, 1,500 tonnes of propan-1-ol were sold. In 1995, the production of propan-1-ol was ceased; the requisite amounts of propan-1-ol for the production of the n-propylamine derivatives are supplied from Bay City, USA (Hoechst AG, 1994 and 1995b).

Based on the available information the following consumption’s of propan-1-ol are estimated for Western EU (CEH, 1995):

- 55% were used as solvent, hereof:
  - approximately 20% to cosmetics,
  - approximately 35% pharmaceuticals (disinfectants),
  - approximately 5% cleaning/washing agents and
  - approximately 5% to other.
• 45% were processed as an intermediate for the production of:
  - approximately 75% to n-propylacetate,
  - approximately 20% to propylchlorformiate and
  - approximately 5% to reactive resins.

Because of the various direct applications of propan-1-ol in end products it has to be expected that the handled amount of propan-1-ol in Europe may increase through import. No further information is available on import or export, as well as on residual content of propan-1-ol in end products.

The use of propan-1-ol in cleaning agents, pesticides, thinners, paints, printing inks and solvents is described in SPIN – Substances in Preparations in the Nordic countries data base. The information contained in SPIN is listed in Table 2.1.

Table 2.1  Information on propan-1-ol in consumer products in the Nordic countries obtained from SPIN data base (July 2003)

<table>
<thead>
<tr>
<th>Country</th>
<th>Year</th>
<th>Number of preparations</th>
<th>Quantity of propan-1-ol contained in preparations [tonnes]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIN</td>
<td>2001</td>
<td>181</td>
<td>3,341</td>
</tr>
<tr>
<td>N</td>
<td>2001</td>
<td>110</td>
<td>2,675</td>
</tr>
<tr>
<td>DK</td>
<td>2001</td>
<td>208</td>
<td>1,925</td>
</tr>
<tr>
<td>S</td>
<td>2000</td>
<td>202</td>
<td>743</td>
</tr>
</tbody>
</table>

The main use categories of the preparations containing propan-1-ol are cleaning/washing agents (N), reprographic agents and solvents (DK), activators and dyestuffs (FIN), solvents and de-icing agents (S). There are also non-industrial sources of propan-1-ol: It is contained in landfill gas; it is formed from plants and animals through putrefaction and decomposition; alcohol-forming bacteria are involved here. The substance is contained in aromas of fruits and other foodstuffs. It is a natural component of alcoholic beverages that have been obtained through fermentation of plant raw materials (GDCh, 1997). The quantity of formed propan-1-ol and the resultant environmental concentration in the different compartments cannot be quantified. However, it is assumed that these are very low and can be neglected.

The following table shows the main, industrial and use categories and the mass balance of propan-1-ol for the EU.

Table 2.2  Use categories and mass balance of propan-1-ol

<table>
<thead>
<tr>
<th>Main category (MC)</th>
<th>Industrial category (IC)</th>
<th>Use category (UC)</th>
<th>Mass balance [in % of use]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-dispersive use (3)</td>
<td>Chemical industry (3)</td>
<td>Intermediate (33)</td>
<td>45</td>
</tr>
<tr>
<td>Non-dispersive use (3)</td>
<td>Other (0)</td>
<td>Solvent (48)</td>
<td>3</td>
</tr>
<tr>
<td>Wide dispersive use (4)</td>
<td>Personal/domestic (5)</td>
<td>Solvent (48)</td>
<td>33</td>
</tr>
<tr>
<td>Wide dispersive use (4)</td>
<td>Paint, lacquers and varnishes industry (14)</td>
<td>Solvent (48)</td>
<td>19</td>
</tr>
</tbody>
</table>

* Sum of quantity used as solvent for cosmetics, pharmaceutics (disinfectants) and cleaning/washing agents.
3 ENVIRONMENT

From the intrinsic properties it is expected that propan-1-ol is of low concern for the environment. Conservative estimates based on worst-case assumptions at the exposure and effects side were used. If the risk assessment performed in that way does not indicate any risk, no further work is considered to be necessary.

3.1 ENVIRONMENTAL EXPOSURE

3.1.1 General discussion

Release into the environment

During production, processing (use as an intermediate), formulation of products (containing propan-1-ol) and further use as a solvent, propan-1-ol is expected to enter the environment via the waste water and the exhaust air.

Degradation

Biodegradation

The biodegradability of propan-1-ol in water has been shown in a number of investigations under most varied conditions. However, no standardised tests for ready biodegradability are available. The most relevant test results for the risk assessment are presented below. Only tests are cited in which propan-1-ol was the only carbon source.

Vaishnav et al. (1987) and Babu and Vaishnav (1987) found a BOD₅/THOD ratio of 60% with an acclimated microbial culture from a domestic sewage (1 ml/bottle).

A BOD₅/COD ratio of 73% was determined with industrial activated sludge (BASF, 1978).

Pitter (1976) achieved an elimination of propan-1-ol of 98.8% measured as COD after 20 days with adapted activated sludge in a concentration of 100 mg/l.

Only one study is available that used unadapted and unacclimated inoculum (Price et al., 1974). In this study BOD/TOD ratios of 64, 76, 81 and 75% were found after 5, 10, 15 and 20 days. As the pass level of 60% as well as the 10-day window criterion was reached in this study, propan-1-ol can be regarded as readily biodegradable.

There are no results from simulation tests for biodegradation in waste water treatment plants, in the aquatic compartment and in soil. Consequently, taking account of the above-mentioned study, the following rate constants may be considered for biodegradation in accordance with the TGD.
Table 3.1 Degradation constants of propan-1-ol in different compartments

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Degradation constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waste water treatment plant</td>
<td>$k_{bio_{WWTP}} = 1 \text{ h}^{-1}$</td>
</tr>
<tr>
<td>Aquatic environment</td>
<td>$k_{bio_{SW}} = 0.047 \text{ d}^{-1}$</td>
</tr>
<tr>
<td>Soil</td>
<td>$k_{bio_{SOL}} = 0.023 \text{ d}^{-1}$</td>
</tr>
<tr>
<td>Sediment</td>
<td>$k_{bio_{SED}} = 0.0023 \text{ d}^{-1}$</td>
</tr>
</tbody>
</table>

(see Appendix A1 for calculation)

**Photodegradation**

Direct photolysis of propan-1-ol in the atmosphere is not to be expected. However, in the atmosphere gaseous propan-1-ol reacts with hydroxyl radicals which are formed photochemically. Wallington and Kurylo (1987) determined a rate constant ($k_{deg_{air}}$) of $5.34 \cdot 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for this reaction at 296 K. Using an atmospheric concentration of the OH-radicals amounting to $5 \cdot 10^5 \text{ OH/cm}^3$, a half-life of 3 days is calculated for the photochemical degradation in the atmosphere.

An estimation of the half-life for the atmospheric reaction of propan-1-ol with hydroxyl radicals with the program AOP 1.65 yields a value of 77.3 h (24-hour day, $5 \cdot 10^5 \text{ OH/cm}^3$). This estimated half-life is used for the further calculations (see Appendix A1 for calculation).

**Hydrolysis and Photolysis**

A direct hydrolysis or photolysis in water is not expected due to the molecular structure of propan-1-ol, i.e. there is no relevant absorption above a wavelength of 290 nm.

**Distribution**

On account of the vapour pressure of 19.4 hPa, propan-1-ol is expected to evaporate quickly from surfaces.

A Henry’s law constant of 0.117 Pa m$^3$/mol at 20°C is calculated from the data on the vapour pressure and water solubility of propan-1-ol given in Section 1. There are some experimentally determined Henry's law constants available in the literature. These vary from 0.377 Pa m$^3$/mol to 0.779 Pa m$^3$/mol (Altschuh et al., 1999; Betterton, 1992; Welke et al., 1998). Checks showed that these measured values although higher than the calculated one have no impact on the distribution in the WWTP. Since data are partly cited from secondary literature only and originating mainly from 1963 to 1985, the calculated Henry's law constant is used further in the RAR. Based on above mentioned data propan-1-ol can be considered as moderately volatile from an aqueous solution. (see Appendices for the calculation).

No bioaccumulation potential is to be expected due to the measured log $P_{ow}$ value of 0.34. Based on this value the $K_{oc}$ is calculated as 4.291 l/kg and the partition coefficients can be calculated according to the organic carbon content in the individual environmental compartments.
### Table 3.2  Partition coefficients of propan-1-ol

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Partition coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil-water</td>
<td>$K_{p_{\text{soil}}}$ = 0.086 l/kg</td>
</tr>
<tr>
<td>Sediment-water</td>
<td>$K_{p_{\text{sed}}}$ = 0.215 l/kg</td>
</tr>
<tr>
<td>Suspended matter-water</td>
<td>$K_{p_{\text{susp}}}$ = 0.429 l/kg</td>
</tr>
<tr>
<td>Sewage sludge-water</td>
<td>$K_{p_{\text{sludge}}}$ = 1.588 l/kg</td>
</tr>
</tbody>
</table>

(see Appendices for the calculation)

The following theoretical distribution is the environment results for propan-1-ol using the distribution model according to Mackay (Level 1) and the physico-chemical properties given in Section 1.

### Table 3.3  Percentage distribution of propan-1-ol

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>3.87</td>
</tr>
<tr>
<td>Water</td>
<td>96.13</td>
</tr>
<tr>
<td>Soil</td>
<td>0.0</td>
</tr>
<tr>
<td>Sediment</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Consequently, the hydrosphere is the target compartment for propan-1-ol in the environment.

### Elimination in waste water treatment plants

Based on the physico-chemical properties of propan-1-ol and in consideration of the rate constant for biodegradation of 0.1 h\(^{-1}\), the elimination in waste water treatment plants can be determined using the SIMPLETREAT model in accordance with the TGD as follows (see Appendices):

### Table 3.4  Elimination in WWTPs

<table>
<thead>
<tr>
<th>Process</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaporation to air (%)</td>
<td>0.1</td>
</tr>
<tr>
<td>Release (dissolved) to water (%)</td>
<td>12.6</td>
</tr>
<tr>
<td>Adsorption to sewage sludge (%)</td>
<td>0</td>
</tr>
<tr>
<td>Degradation (%)</td>
<td>87.3</td>
</tr>
<tr>
<td>Total elimination from water (%)</td>
<td>87.4</td>
</tr>
</tbody>
</table>

### Accumulation

No investigations on bioaccumulation are available. The measured log $P_{\text{ow}}$ of 0.34 does not provide any indication of a relevant bioaccumulation potential.

The calculated $K_{\text{oc}}$ value of 4.29 l/kg (see Appendix A1 for the calculation) also does not indicate that a significant geoaccumulation potential is to be expected for propan-1-ol. The substance may be washed out from soil to groundwater by rainwater depending on the elimination in soil by degradation and distribution.
3.1.2 **Aquatic compartment**

Releases into the waste water occur during production, use as an intermediate and use in products. The exposure data submitted by the company for production of propan-1-ol is used for the calculation of environmental concentration of propan-1-ol in surface water.

Since no exposure data have been submitted by the companies for further processing of propan-1-ol, in accordance with the ESD (Emission Scenario Documents, TGD Chapter 7), releases into the waste water amounting to 0.7% of the processing quantity are considered.

The exposure scenario for the formulation and use of propan-1-ol in products is based on the A and B Tables of the TGD.

3.1.2.1 **Determination of the C\text{local}\text{water} / generic approach with regard to production and use as an intermediate**

A generic exposure scenario for the entry of propan-1-ol into the waste water during production is not used because the producer has submitted the necessary exposure information.

Taking into consideration a maximum processing quantity at one site of 5,000 tonnes/annum (typical quantity for a company) a $C_{\text{local}\text{water}}$ of approximately 2.84 µg/l results for use of propan-1-ol as an intermediate at one processing site (see Appendices for the calculation, river flow rate = 60 m$^3$ s$^{-1}$).

3.1.2.2 **Determination of the C\text{local}\text{water} / site-specific approach with regard to production**

Using the currently available information on the individual manufacturer, site specific exposure calculation can be performed for this site (BASF AG, 1996).

Recently provided monitoring data (364 individual measurements in waste water effluent from 2000, 90 percentile) result in a $C_{\text{local}\text{water}}$ of 0.14 µg/l for the producer of propan-1-ol in the EU (see Appendices for the calculation).

3.1.2.3 **Determination of the C\text{local}\text{water} / generic approach: use**

Propan-1-ol is used as a solvent for disinfectants, pharmaceutical products, cleaning agents, paints, coating materials, enamel and lacquer paints, printing inks and cosmetics. The quantitative distribution of the application areas described in Section 2.2 is used for the exposure assessment.

A total amount of ca. 16,600 tonnes/annum is used as a solvent in the EU. Since it can be assumed that there are a large number of formulators and users involved, the 10% rule is applied to the calculation of $C_{\text{local}\text{water}}$ for these life cycles. The following quantities are considered for the calculation of the $C_{\text{local}\text{water}}$. 
Table 3.5 Use quantities of propan-1-ol as solvent within EU

<table>
<thead>
<tr>
<th>Application</th>
<th>Distribution</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>cosmetics</td>
<td>20%</td>
<td>9,960 tonnes/annum</td>
</tr>
<tr>
<td>pharmaceutics (disinfectants)</td>
<td>35%</td>
<td></td>
</tr>
<tr>
<td>cleaning/washing agents</td>
<td>5%</td>
<td>5,810 tonnes/annum</td>
</tr>
<tr>
<td>for IC 5 (personal/domestic)</td>
<td>60%</td>
<td>9,960 tonnes/annum</td>
</tr>
<tr>
<td>for IC 14 (lacquer, paints)</td>
<td>35%</td>
<td>5,810 tonnes/annum</td>
</tr>
</tbody>
</table>
| for IC 0 (other)                           | 5%           | 830 tonnes/annum  

Use as a solvent in cosmetics, pharmaceutics (disinfectants) and cleaning/washing agents

If the substance is used as a solvent in cosmetics, pharmaceutics (disinfectants) and cleaning/washing agents, exposure is to be expected during the formulation of the products in the relevant companies. In addition, releases are expected during use of the products.

For the release estimations based on the use of propan-1-ol as a solvent in cosmetics, pharmaceutics (disinfectants) and cleaning/washing agents it is assumed that these 3 use categories are summarised for the formulation in companies and for the use as products in private households. This assumption is the conservative “worst case” and is used for the exposure calculation on the basis of default values.

The product quantity is estimated according to different fields of application (input B Tables).

Table 3.6 Estimation of product quantities containing propan-1-ol

<table>
<thead>
<tr>
<th>application</th>
<th>quantity of used propan-1-ol</th>
<th>concentration in products</th>
<th>quantity of products</th>
</tr>
</thead>
<tbody>
<tr>
<td>cosmetics</td>
<td>3,320 tonnes/annum</td>
<td>10%</td>
<td>33,200 tonnes/annum</td>
</tr>
<tr>
<td>pharmaceutics (disinfectants)</td>
<td>5,810 tonnes/annum</td>
<td>25%</td>
<td>23,240 tonnes/annum</td>
</tr>
<tr>
<td>cleaning/washing agents</td>
<td>830 tonnes/annum</td>
<td>15%</td>
<td>5,530 tonnes/annum</td>
</tr>
<tr>
<td>total quantity</td>
<td>9,960 tonnes/annum</td>
<td>-</td>
<td>Approximately 61,970 tonnes/annum</td>
</tr>
</tbody>
</table>

In the case of use as a solvent in different products it is assumed that the total quantity used is released either to household waste water or to the atmosphere as a result of evaporation.

Use as a solvent in paints and lacquers

If the substance is used as a solvent in paints and lacquers exposure is to be expected during the formulation of the final products in the relevant companies. In addition, releases are expected during use of the paints and lacquers.

For the release estimations based on the use of propan-1-ol as a solvent in paints and lacquers a content of 50 % of the substance in the products is used for the derivation of the fraction of main source (input B Table) for the formulation of the products. The use of propan-1-ol in solvent based products specified as quick-drying paints and lacquers is assumed.

In the risk assessment the “worst case” exposure scenarios for both, paints for private and industrial use are calculated side by side (based on the used quantity of 5,810 tonnes/annum). With these two calculations one can identify the exposure scenario, leading to the maximum Clocalwater. For the continental and regional exposure calculation only the private use is taken
into consideration (based on the maximum release of propan-1-ol to the environment). There is no information to be able to assign the total volume to one of these two uses.

Use as a solvent in other non specified products

If the substance is used as a solvent for different non specified products exposure is to be expected during the formulation of the final products in the relevant companies. In addition, releases are expected during use of the solvent.

For the release estimations based on the use of propan-1-ol as a solvent a content of approximately 100% of the substance in the products are used for the derivation of the fraction of main source (input B Table) for the formulation (manufacture) of the products. The use of propan-1-ol as solvent is located in industrial area.

The results of the calculations of the C\text{localwater} are summarised in the following table. Since it can be assumed that there are a large number of formulators and users involved, the 10% rule is applied to the calculation of C\text{localwater} in these solvent scenarios.
Table 3.7  Results of calculations of Clocal\textsubscript{water} according to TGD for use of propan-1-ol as solvent

<table>
<thead>
<tr>
<th>Types of use</th>
<th>Solvent in household chemicals (pharmaceutics, disinfectants, cosmetics and cleaning / washing agents)</th>
<th>Solvent in paints and lacquers</th>
<th>Solvent not specified</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tonnage ( a) ) (t/a)</td>
<td>1,000</td>
<td>600</td>
<td>100</td>
</tr>
<tr>
<td>Main category</td>
<td>non-dispersive use (3)</td>
<td>wide dispersive use</td>
<td>non-dispersive use (3)</td>
</tr>
<tr>
<td>Industrial category</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Use category</td>
<td>5 (personal/domestic) 48 (solvents)</td>
<td>14 (paints) 48 (solvents)</td>
<td>14 (paints) 48 (solvents)</td>
</tr>
<tr>
<td>Life cycle step</td>
<td>formulation private use</td>
<td>formulation private use</td>
<td>formulation processing</td>
</tr>
<tr>
<td>Number of days</td>
<td>300 (B-table 2.1)</td>
<td>300 (B-table 2.10)</td>
<td>200 (B-table 2.8)</td>
</tr>
<tr>
<td>Release factor to water</td>
<td>0.003 (A-table 2.1)</td>
<td>0.02 (A-table 2.10)</td>
<td>0.02 (A-table 3.13)</td>
</tr>
<tr>
<td>Fraction of main source</td>
<td>0.4 (B-table 2.3)</td>
<td>0.002 (B-table 4.1)</td>
<td>0.15 (B-table 3.13)</td>
</tr>
<tr>
<td>total emission to waste water (t/a)</td>
<td>3</td>
<td>12</td>
<td>2</td>
</tr>
<tr>
<td>Size of STP (m\textsuperscript{3}/d)</td>
<td>2,000</td>
<td>2,000</td>
<td>2,000</td>
</tr>
<tr>
<td>Dilution in receive. water</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Clocal\textsubscript{effluent} (mg/l)</td>
<td>0.252</td>
<td>2.52</td>
<td>0.38</td>
</tr>
<tr>
<td>Clocal\textsubscript{water} (µg/l)</td>
<td>25.2</td>
<td>252</td>
<td>37.8</td>
</tr>
</tbody>
</table>

\( a) \) Tonnages result from application of 10\% rule. See Appendices for the calculation.
3.1.2.4 Data on occurrence in the hydrosphere

No measured values relating to the occurrence of propan-1-ol in the hydrosphere are available.

3.1.2.5 Sediment

Data on the occurrence in sediment do not exist for propan-1-ol. According to the known physico-chemical properties, there is no indication that propan-1-ol accumulates in sediment.

3.1.3 Atmosphere

In the case of the production of propan-1-ol in the EU, the release into the atmosphere is estimated as being 0.8 tonnes/annum (BASF AG, 1996). No further information is available with regard to the release into the atmosphere during the processing, formulation and use of the substance.

Since no exposure data have been submitted by the companies for further processing and formulation of propan-1-ol, the releases into the atmosphere are calculated in accordance with the TGD (A and B Tables in Chapter 3 Appendix I).

Using the SIMPLETEAT model, with regard to propan-1-ol, release from industrial waste water treatment plants as a result of evaporation into the air is estimated as approximately 0.1% of the quantity of the substance entering the waste water treatment plant. Consequently, an additional release into the atmosphere results for the individual production and processing and formulation sites. The same release route is also to be expected for use of the substance.

Based on the site specific exposure data of the one production site in the EU the resultant air concentration of 0.74 µg/m³ and deposition quantity of 0.89 µg/m²/day are calculated (see Appendices for the calculation).

For the further processing of approximately 5,000 tonnes/annum propan-1-ol at one site (typical quantity for a company) the resultant air concentration of 116 µg/m³ and deposition quantity of 137 µg/m²/day are calculated based on the A and B Tables of the TGD (see Appendices for the calculation).

By taking into consideration the current formulation quantities, the exposure tables in Chapter 3, Appendix I of the TGD and the SIMPLETEAT model, it is possible to calculate the releases into the atmosphere and the resultant deposition quantities according to the physico-chemical properties of the substance and the quantities of it which are used. The results of the calculations are summarised in the following table.

Please note, that releases resulting from use of propan-1-ol in household chemicals are expected mainly to waste water. Although environmental exposure is possible this route is neglected in the assessment.
### Table 3.8 Results of calculations of $C_{localair}$ and $DEP_{totalann}$, according to TGD for use of propan-1-ol as solvent

<table>
<thead>
<tr>
<th>Types of use</th>
<th>Solvent in household chemicals (pharmaceutics, disinfectants, cosmetics and cleaning / washing agents)</th>
<th>Solvent in paints and lacquers</th>
<th>Solvent not specified</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tonnage a) (t/a)</td>
<td>1,000</td>
<td>1,000</td>
<td>600</td>
</tr>
<tr>
<td>Main category</td>
<td>non-dispersive use (3)</td>
<td>wide dispersive use</td>
<td>non-dispersive use (3)</td>
</tr>
<tr>
<td>Industrial category</td>
<td>5 (personal/domestic)</td>
<td>48 (solvents)</td>
<td>14 (paints)</td>
</tr>
<tr>
<td>Use category</td>
<td></td>
<td></td>
<td>48 (solvents)</td>
</tr>
<tr>
<td>Life cycle step</td>
<td>formulation</td>
<td>private use</td>
<td>formulation</td>
</tr>
<tr>
<td>Number of days</td>
<td>300 (B-table 2.1)</td>
<td>300 (B-table 2.10)</td>
<td>300 (B-table 4.5)</td>
</tr>
<tr>
<td>Release factor to air</td>
<td>0.025 (A-table 2.1)</td>
<td>0.025 (A-table 2.1)</td>
<td>0.95 (A-table 4.5)</td>
</tr>
<tr>
<td>Fraction of main source</td>
<td>0.4 (B-table 2.1)</td>
<td>1 (B-table 2.10)</td>
<td>0.0004 (B-table 4.5)</td>
</tr>
<tr>
<td>Direct emission to air (t/a)</td>
<td>25</td>
<td>15</td>
<td>5,520</td>
</tr>
<tr>
<td>Annual deposition (µg/m²d)</td>
<td>11</td>
<td>16</td>
<td>0.25</td>
</tr>
<tr>
<td>$C_{localair}$ (µg/m³)</td>
<td>9.3</td>
<td>14</td>
<td>0.21</td>
</tr>
</tbody>
</table>

a) Tonnages result from application of 10% rule.

See Appendix A4 for the calculation.
3.1.4 Terrestrial compartment

Propan-1-ol is expected to enter the soil as a result of deposition from the atmosphere. In this regard, the point sources of the production and the use of the substance as an intermediate as well as a solvent involving the highest amount of air pollution are considered (see Section 3.1.3). The release of propan-1-ol to the soil according to these scenarios are summarised in the following table.

<table>
<thead>
<tr>
<th>Type of use</th>
<th>Route of exposure</th>
<th>PEC_{local \text{soil-pore}} in µg/l</th>
<th>C_{local \text{soil}} in µg/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Production</td>
<td>deposition</td>
<td>3.15</td>
<td>0.08</td>
</tr>
<tr>
<td>Processing of 5,000 t/a at one site</td>
<td>deposition</td>
<td>69.1</td>
<td>12.9</td>
</tr>
<tr>
<td>(typical quantity for a company)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Formulation of household chemicals</td>
<td>deposition</td>
<td>8.04</td>
<td>1.03</td>
</tr>
<tr>
<td>Processing of paints in paint shops</td>
<td>deposition</td>
<td>45.8</td>
<td>8.35</td>
</tr>
<tr>
<td>Formulation of solvents (not specified)</td>
<td>deposition</td>
<td>4.04</td>
<td>0.26</td>
</tr>
</tbody>
</table>

See Appendices for the calculation.

Based on the SIMPLETREAT model (see Section 3.1.1) there is no adsorption of propan-1-ol at sewage sludge to be expected and the release to soil with sewage sludge application in agriculture is not considered in the risk assessment.

3.1.5 Secondary poisoning

Since there is no indication of propan-1-ol possessing a bioaccumulation potential, a risk characterisation for exposure via the food chain is not necessary.

3.1.6 Other non industrial emissions of propan-1-ol

Propan-1-ol is contained in landfill gas; it is formed from plants and animals through putrefaction and decomposition; alcohol-forming bacteria are involved here. The substance is contained in aromas of fruits and other foodstuffs. It is a natural component of alcoholic beverages that have been obtained through fermentation of plant raw materials (GDCh, 1997).

The quantity of formed propan-1-ol and the resultant environmental concentration in the different compartments cannot be quantified.

3.1.7 Regional exposure consideration

One production site and a processing site with a capacity of 5,000 tonnes/annum propan-1-ol (typical quantity for a company) are located in the considered region. The emission from the processing of the remaining approximately 8,500 tonnes/annum propan-1-ol is located in the continent.
In the determination of a regional background concentration all releases, from point and diffuse sources of the formulation and use of propan-1-ol, are considered. Two third (67%) of the total exposure quantity are taken into account for the continental model and one third (33%) of it for the defined regional EU standard model (densely populated area of 200 × 200 km with 20 million inhabitants). This conservative assumption is used for the first exposure assessment.

No direct release into the soil was identified. Diffuse release only occurs as a result of dispersal processes. Release is therefore to be expected as a result of deposition from the air (see Section 3.1.4).

Information is available according to which approximately 55% of the production volume is used as a solvent. Releases into the hydrosphere (see Section 3.1.2.3) and the atmosphere (see Section 3.1.3) are to be expected here.

Since not all of the previously mentioned releases arising from use of the substance enter the hydrosphere directly, but instead primarily via the waste water which is possibly purified in municipal waste water treatment plants, a 70% connection to waste water treatment plants, in which 67.4% of the substance is biodegraded and 0.1% volatilised, is assumed for this scenario. The remaining 30% of the water is discharged directly into the hydrosphere.

The individual environmental releases are summarised in the following table.

<table>
<thead>
<tr>
<th>field of application</th>
<th>Ratio reg./cont.</th>
<th>release to WWTPs (t/a)</th>
<th>direct release to the hydrosphere (t/a)</th>
<th>release into the atmosphere (t/a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>production</td>
<td>100/0</td>
<td>9.8</td>
<td>-</td>
<td>0.8</td>
</tr>
<tr>
<td>use as intermediate approx. 13,500 t/a</td>
<td>37/63</td>
<td>94.5</td>
<td>-</td>
<td>337.5</td>
</tr>
<tr>
<td>formulation of household chemicals</td>
<td>33/67</td>
<td>30</td>
<td>-</td>
<td>249</td>
</tr>
<tr>
<td>private use of household chemicals</td>
<td>33/67</td>
<td>4,186</td>
<td>1,794</td>
<td>-</td>
</tr>
<tr>
<td>formulation of paints</td>
<td>33/67</td>
<td>17.4</td>
<td>-</td>
<td>145.3</td>
</tr>
<tr>
<td>private use of paints</td>
<td>33/67</td>
<td>162.4</td>
<td>69.6</td>
<td>5,520</td>
</tr>
<tr>
<td>processing of paints*</td>
<td>(33/67)</td>
<td>(116)</td>
<td>(-)</td>
<td>(5,229)</td>
</tr>
<tr>
<td>formulation of solvents (not specified)</td>
<td>33/67</td>
<td>16.6</td>
<td>-</td>
<td>20.8</td>
</tr>
<tr>
<td>use of solvents (not specified)</td>
<td>33/67</td>
<td>8.3</td>
<td>-</td>
<td>8.3</td>
</tr>
<tr>
<td>total</td>
<td>-</td>
<td>4,525</td>
<td>1,864</td>
<td>6,282</td>
</tr>
</tbody>
</table>

* Not considered for the regional PEC, since the more release-relevant life-cycle stage "private use of paints" is already involved

In the calculation for the continental and regional model the individual releases are as follows.
Table 3.11 Input data for calculation of regional and continental PECs

<table>
<thead>
<tr>
<th></th>
<th>continental model</th>
<th>regional model</th>
</tr>
</thead>
<tbody>
<tr>
<td>to air</td>
<td>4,174</td>
<td>2,107</td>
</tr>
<tr>
<td>to soil</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>to hydrosphere (direct)</td>
<td>1,249</td>
<td>615</td>
</tr>
<tr>
<td>to WWTPs</td>
<td>3,016</td>
<td>1,509</td>
</tr>
</tbody>
</table>

The figures given in the tables above were included exactly as they were estimated in the previous sections in order to ensure comprehensibility. The exactitude of the figures is not, however, intended as an indication of the absolute correctness.

The regional PECs resulting from the SimpleBox 2.0 calculations are (further details are presented in the Appendix A6):

\[
\begin{align*}
\text{PEC}_{\text{regional, water}} & = 8.59 \, \mu g/l \\
\text{PEC}_{\text{regional, soil}} & = 0.525 \, \mu g/kg \\
\text{PEC}_{\text{regional, air}} & = 94.5 \, \text{ng/m}^3
\end{align*}
\]

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

3.2.1 Aquatic compartment

Available effect data

The propan-1-ol short-term toxicity studies to fish are summarised in the following table.

Table 3.12 Short-term toxicity to vertebrates

<table>
<thead>
<tr>
<th>Test organism</th>
<th>Criterion</th>
<th>Duration [h]</th>
<th>Test system</th>
<th>Result [mg/l]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Oncorhynchus mykiss</em></td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC\text{50} = 3,200 (n)</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Pimephales promelas</em></td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC\text{50} = 5,000 (n)</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Oryzias latipes</em></td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC\text{50} = 5,900 (n)</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Leuciscus idus melanotus</em></td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC\text{50} = 4,320 (n)</td>
<td>Juhnke/ Lüdemann 1978</td>
</tr>
<tr>
<td><em>Leuciscus idus melanotus</em></td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC\text{50} = 4,560 (n)</td>
<td>Juhnke/ Lüdemann 1978</td>
</tr>
<tr>
<td><em>Pimephales promelas</em></td>
<td>Mortality</td>
<td>96</td>
<td>flow-through</td>
<td>LC\text{50} = 4,480 (m)</td>
<td>Brooke et al. 1984</td>
</tr>
<tr>
<td><em>Pimephales promelas</em></td>
<td>Mortality</td>
<td>96</td>
<td>flow-through</td>
<td>LC\text{50} = 4,630 (m)</td>
<td>Brooke et al. 1984</td>
</tr>
<tr>
<td><em>Alburnus alburnus</em></td>
<td>Mortality</td>
<td>96</td>
<td>flow-through</td>
<td>LC\text{50} = 3,800 (n)</td>
<td>Bengtsson et al. 1984</td>
</tr>
</tbody>
</table>

Table 3.12 continued overleaf
### Table 3.12 continued Short-term toxicity to vertebrates

<table>
<thead>
<tr>
<th>Test organism</th>
<th>Criterion</th>
<th>Duration [h]</th>
<th>Test system</th>
<th>Result [mg/l]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oryzias latipes</td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC50 &gt; 1,000 (n) (T: 10°C, 20°C) LC50 = 640 (n) (T: 30°C)</td>
<td>Tsuji et al. 1986</td>
</tr>
<tr>
<td>Ambystoma mexicanum</td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC50 = 4,000 (n)</td>
<td>Slooff/Baerselman 1980</td>
</tr>
<tr>
<td>Xenopus laevis</td>
<td>Mortality</td>
<td>48</td>
<td>static</td>
<td>LC50 = 4,000 (n)</td>
<td>Slooff/Baerselman 1980</td>
</tr>
</tbody>
</table>

n nominal; m measured

The reported effect values for fish show similar sensitivity of the tested species without considerable influence of the exposure duration (48 or 96 hours). Most tests were performed in open static systems without analytical monitoring of the test substance concentration. As propan-1-ol is moderately volatile (Henry’s law constant 0.117 Pa m³/mol) it cannot be excluded that a decrease in test substance concentration may have occurred and the real effect values are therefore lower. However, from the two tests performed in flow-through systems with analytical monitoring, that found effect values in the same order of magnitude like the other available tests, it can be concluded that volatilisation will not have influenced the test results to a great extent.

Generally the observed effects reveal no serious toxicity of propan-1-ol to fish and amphibians. The lowest reported LC50-value for fish was 640 mg/l. However, as this value was found at a temperature of 30°C it is not used for the further risk assessment. Instead, the value of 3,200 mg/l found for *Oncorhynchus mykiss* is interpreted as lowest available effect value for fish.

The following table shows the propan-1-ol short-term toxicity studies for invertebrates.

### Table 3.13 Short-term toxicity to invertebrates

<table>
<thead>
<tr>
<th>Test organism</th>
<th>Criterion</th>
<th>Duration [h]</th>
<th>Result [mg/l]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Daphnia magna</em></td>
<td>Immobilisation</td>
<td>24</td>
<td>EC50 = 4,262 EC50 = 3,644</td>
<td>Kühn et al. 1989</td>
</tr>
<tr>
<td><em>Daphnia magna</em></td>
<td>Immobilisation</td>
<td>48</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Artemia salina</em></td>
<td>Mortality</td>
<td>24</td>
<td>LC50 = 4,200</td>
<td>Price 1974</td>
</tr>
<tr>
<td><em>Gammarus pulex</em></td>
<td>Mortality</td>
<td>48</td>
<td>EC50 = 1,000</td>
<td>Slooff 1983</td>
</tr>
<tr>
<td><em>Corixa punctata</em></td>
<td>Mortality</td>
<td>48</td>
<td>EC50 = 2,000</td>
<td>Slooff 1983</td>
</tr>
<tr>
<td><em>Ischnura elegans</em></td>
<td>Mortality</td>
<td>48</td>
<td>LC50 = 4,200</td>
<td>Slooff 1983</td>
</tr>
<tr>
<td><em>Nemoura cinerea</em></td>
<td>Mortality</td>
<td>48</td>
<td>LC50 = 1,520</td>
<td>Slooff 1983</td>
</tr>
<tr>
<td><em>Erpobdella octoculata</em></td>
<td>Mortality</td>
<td>48</td>
<td>LC50 = 1,400</td>
<td>Slooff 1983</td>
</tr>
<tr>
<td><em>Nitocra spinipes</em></td>
<td>Mortality</td>
<td>96</td>
<td>LC50 = 2,300</td>
<td>Bengtsson et al. 1984</td>
</tr>
</tbody>
</table>
All tests were performed without analytical monitoring of the test substance concentration. As discussed above, no significant decrease in test substance concentration due to volatilisation is expected. The lowest effect value of 1,000 mg/l was found for *Gammarus pulex*.

The following table shows the toxicity of propan-1-ol to different algae species. The results are given as nominal concentrations.

**Table 3.14 Toxicity to algae**

<table>
<thead>
<tr>
<th>Test organism</th>
<th>Criterion</th>
<th>Duration [h]</th>
<th>Result [mg/l]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Selenastrum capricornutum</em></td>
<td>Growth</td>
<td>96</td>
<td>NOEC = 2,000</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Scenedesmus pannonicus</em></td>
<td>Growth</td>
<td>48</td>
<td>NOEC = 2,900</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Chlorella pyrenoidosa</em></td>
<td>Growth</td>
<td>48</td>
<td>NOEC = 1,150</td>
<td>Slooff et al. 1983</td>
</tr>
<tr>
<td><em>Microcystis aeruginosa</em></td>
<td>Cell multiplication inhibition</td>
<td>192</td>
<td>TTC = 255</td>
<td>Bringmann 1975</td>
</tr>
<tr>
<td><em>Scenedesmus quadricauda</em></td>
<td>Cell multiplication inhibition</td>
<td>192</td>
<td>TTC = 3,100</td>
<td>Bringmann/ Kühn 1977b</td>
</tr>
</tbody>
</table>

All tests were performed in open systems without analytical monitoring of the test substance concentration. Again, as discussed above it is not expected that the concentration of propan-1-ol significantly decreases due to volatilisation. Only NOEC-values or toxic threshold concentrations are available. The lowest TTC of 255 mg/l was found in a test with the blue-green algae *Microcystis aeruginosa*. However, due to the long exposure period of 8 days it can be assumed the growth of the algal culture is no longer in the exponential phase and therefore the test is regarded as not valid. The same is true for the 192-hour test with *Scenedesmus quadricauda*. Therefore, the lowest valid effect value for algae is the NOEC of 1,150 mg/l found for *Chlorella pyrenoidosa*.

The propan-1-ol microbial toxicity studies are shown in the following table.

**Table 3.15 Toxicity to microorganisms**

<table>
<thead>
<tr>
<th>Test organism</th>
<th>Criterion</th>
<th>Duration [h]</th>
<th>Result [mg/l]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activated sludge</td>
<td>Resp. inhibition</td>
<td>12</td>
<td>EC50 = 9,600 (closed system)</td>
<td>Blum/Speece 1991</td>
</tr>
<tr>
<td>Nitrosomonas sp.</td>
<td>Inhibition of ammonia consumption</td>
<td>12</td>
<td>EC50 = 980 (closed system)</td>
<td>Blum/Speece 1991</td>
</tr>
<tr>
<td>Methanogens</td>
<td>Inhibition of gas production</td>
<td>12</td>
<td>EC50 = 34,000 (closed system)</td>
<td>Blum/Speece 1991</td>
</tr>
<tr>
<td>Activated sludge (municipal)</td>
<td>Resp. inhibition</td>
<td>3</td>
<td>IC50 &gt; 1,000</td>
<td>Klecka et al. 1985</td>
</tr>
<tr>
<td><em>Pseudomonas putida</em></td>
<td>Resp. inhibition</td>
<td>0.5</td>
<td>EC50 = 11,421</td>
<td>Robra 1979</td>
</tr>
<tr>
<td><em>Pseudomonas putida</em></td>
<td>Cell multiplication</td>
<td>16</td>
<td>TTC = 2,700</td>
<td>Bringmann/ Kühn 1977b</td>
</tr>
<tr>
<td><em>Entosiphon sulcatum</em></td>
<td>Cell multiplication</td>
<td>72</td>
<td>TTC = 38</td>
<td>Bringmann 1978</td>
</tr>
<tr>
<td><em>Uronema parduczi</em></td>
<td>Cell multiplication</td>
<td>20</td>
<td>TTC = 568</td>
<td>Bringmann/ Kühn 1980</td>
</tr>
<tr>
<td><em>Chilomonas paramecium</em></td>
<td>Cell multiplication</td>
<td>48</td>
<td>TTC = 175</td>
<td>Bringmann et al. 1980</td>
</tr>
</tbody>
</table>
Determination of PNEC\textsubscript{aqua}

The lowest available effect value of 1,000 mg/l was obtained with the invertebrate species \textit{Gammarus pulex}. As no long-term tests with invertebrates and fish are available, an assessment factor of 1,000 has normally to be applied for the PNEC derivation. However, according to the TGD the usage of a lower assessment factor of 100 is justified because a) data from a wide selection of species covering additional taxonomic groups other than those represented by the base-set species (e.g. amphibians) are available (which additionally cross three trophic levels) and b) the mode of action law can be implemented (non-polar narcosis).

Therefore: \( PNEC\textsubscript{aqua} = \frac{1,000 \text{ mg/l}}{100} = 10 \text{ mg/l} \)

Determination of PNEC\textsubscript{microorganisms}

The most sensitive species to propan-1-ol was the protozoan \textit{Entosiphon sulcatum}. However, the TTC of 38 mg/l found with this species is not used for the derivation of the PNEC\textsubscript{microorganisms} as \textit{Entosiphon sulcatum} is not a typical representative of sewage treatment plants. The application of the following assessment factors according to the TGD to the other lowest available effect values gives the following PNEC\textsubscript{microorganisms}:

<table>
<thead>
<tr>
<th>Organism</th>
<th>TTC / IC50</th>
<th>AF</th>
<th>PNEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chilomonas paramaecium</td>
<td>175 mg/l</td>
<td>1</td>
<td>175 mg/l</td>
</tr>
<tr>
<td>Activated sludge</td>
<td>IC50 = 9,600 mg/l</td>
<td>100</td>
<td>96 mg/l</td>
</tr>
<tr>
<td>Nitrosomonas sp</td>
<td>IC50 = 980 mg/l</td>
<td>10</td>
<td>98 mg/l</td>
</tr>
<tr>
<td>Pseudomonas putida</td>
<td>TTC = 2,700 mg/l</td>
<td>1</td>
<td>2,700 mg/l</td>
</tr>
</tbody>
</table>

The PNEC derived from the effect values of activated sludge and \textit{Nitrosomonas} are in the same order. The lowest derived value is 96 mg/l.

Therefore: \( PNEC\textsubscript{microorganisms} = 96 \text{ mg/l} \)

Sediment

No risk assessment is required for this compartment since there are no indications of adsorption of the substance to sediments and neither measured concentrations of propan-1-ol for sediments nor experimental investigations with sediment organisms are available.

3.2.2 Atmosphere

No ecotoxicological data are available for this environmental compartment.

3.2.3 Terrestrial compartment

No ecotoxicological data are available for terrestrial organisms. In approximation, the aquatic PNEC can be used for the purpose of a risk assessment for the terrestrial compartment and compared with the concentration determined for the soil pore water:

\[ PNEC\textsubscript{soil} = 10 \text{ mg/l (soil pore water)} \]
3.2.4 Secondary Poisoning

Since propan-1-ol does not possess a bioaccumulation potential and is neither classified as “toxic” nor “harmful”, it is not necessary for a PNEC to be derived.

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment

Waste water treatment plants

The highest discharge concentration for waste water treatment plants is calculated as 2.52 mg/l for the formulation of solvents in paints and lacquers. A value of 1.58 mg/l was derived for the industrial processing of solvents (not specified); all other Clocal_{eff} are in the µg/l range. Generic models are used for the calculation of the Clocal_{eff}, since no specific information is available.

Taking into consideration a PNEC_{microorganisms} of 96 mg/l, maximum Clocal_{eff}/PNEC ratios of 0.03 and ~0.02 result for these life cycle steps of propan-1-ol. Since the Clocal_{eff}/PNEC ratios < 1, there is no risk to the microorganism population in the WWTP. **Conclusion (ii).**

Aquatic environments

The PEC/PNEC ratios for all of the areas of production, processing and use are summarised in the following table (PEC_{regional}= 8.59 µg/l; PNEC_{aqua}= 10 mg/l).

<table>
<thead>
<tr>
<th>Company/area of use</th>
<th>PEC_{local} [µg/l]</th>
<th>PEC/PNEC_{aqua}</th>
</tr>
</thead>
</table>
| • Production at Site – A  
  • Use as intermediate at Site - B  
  (typical quantity for a company) | 8.73  
  11.4 | < 0.01  
  < 0.01 |
| Formulation of household chemicals  
  (used as a solvent in cosmetics, pharmaceutics, disinfectants and cleaning/washing agents) | 33.8 | < 0.01 |
| Use of household chemicals  
  (used as a solvent in cosmetics, pharmaceutics, disinfectants and cleaning/washing agents) | 29.3 | < 0.01 |
| Formulation of paints | 261 | 0.03 |
| Use of paints in the private domain | 8.79 | < 0.01 |
| Processing of paints in paint shops  
  (e.g. car painting) | 46.4 | < 0.01 |
| Formulation of solvents  
  (for industrial use) | 71.6 | < 0.01 |
| Processing of solvents  
  (for industrial use) | 166 | 0.02 |

Based on the conservative approaches for the exposure assessment all PEC/PNEC ratios < 1. On the currently available data there is no risk to aquatic organisms. **Conclusion (ii).**
Sediment

No data on the occurrence in sediment or investigations of the effect on benthic organisms are available in connection with propan-1-ol. According to the available physico-chemical properties of the substance, there is no indication that propan-1-ol accumulates in sediment. Consequently, there is no need for a risk consideration for this compartment. **Conclusion (ii).**

### 3.3.2 Atmosphere

Due to the atmospheric half-life ($t_{1/2} = $ approximately 77 hours), abiotic effects on the atmosphere, such as global warming and ozone depletion, are not to be expected in connection with propan-1-ol. The highest calculated air concentration is around 75 µg/m³ for the processing of paints in paint shops (propan-1-ol is used as a solvent). Since no data are available on the ecotoxicological effect of the substance in connection with this environmental compartment, it is not possible to undertake a quantitative assessment of this environmental compartment. On the basis of the available information on the substance, the performance of tests is not considered necessary. **Conclusion (ii).**

### 3.3.3 Terrestrial compartment

Releases into the terrestrial compartment as a result of deposition from the atmosphere are to be expected. The highest deposition rates result from the processing of propan-1-ol (generic approach) and the processing of paints in paint shops (propan-1-ol is used as a solvent). Soil concentrations for propan-1-ol amounting to:

- Processing (generic) 13 µg/kg and 70 µg/l soil pore water
- Processing (paints) 8.4 µg/kg and 47 µg/l soil pore water.

Since no ecotoxicological data are available for terrestrial organisms, in approximation, the aquatic PNEC (10,000 µg/l) is considered for the purpose of the risk assessment of the terrestrial compartment and compared with the concentration determined for the soil pore water. With these data a maximum PEC/PNEC ratio of $< 0.01$ is calculated. Therefore, there is no indication of a risk to the terrestrial environmental compartment at present. **Conclusion (ii).**

### 3.3.4 Secondary poisoning

Since there is no indication that propan-1-ol possesses a bioaccumulation potential, a risk characterisation for exposure via the food chain is not necessary.
4 HUMAN HEALTH

4.1 HUMAN HEALTH (TOXICITY)

4.1.1 Exposure assessment

4.1.1.1 General discussion

4.1.1.2 Occupational exposure

4.1.1.3 Consumer exposure

4.1.1.4 Indirect exposure via the environment

In accordance with the TGD, the indirect exposure of man to propan-1-ol via the environment, e.g. via food, drinking water and air, must be determined. In the form of a worst-case scenario, the most significant point source (in this case: propan-1-ol as solvent; processing of paints) is considered for calculation purposes. This result is then compared with a second calculation which is based on the regional background concentrations (see Section 3.1.7).

The results of these calculations with the corresponding input values are summarised in the Appendices. It is necessary to note, however, that the calculation model applied is as yet only provisional. It requires revision as soon as further information is available.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Local scenario</th>
<th>Regional scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual average PEC in surface water (^1) [mg/l]</td>
<td>0.040</td>
<td>8.59 (\cdot) 10(^{-3})</td>
</tr>
<tr>
<td>Annual average PEC in air (^1) [mg/m(^3)]</td>
<td>0.062</td>
<td>9.45 (\cdot) 10(^{-4})</td>
</tr>
<tr>
<td>PEC in grassland [mg/kg]</td>
<td>0.014</td>
<td>-</td>
</tr>
<tr>
<td>PEC in agricultural soil [mg/kg]</td>
<td>-</td>
<td>2.91 (\cdot) 10(^{4})</td>
</tr>
<tr>
<td>PEC in porewater of agricultural soil [mg/l]</td>
<td>0.046</td>
<td>1.50 (\cdot) 10(^{3})</td>
</tr>
<tr>
<td>PEC in porewater of grassland [mg/l]</td>
<td>0.071</td>
<td>-</td>
</tr>
<tr>
<td>PEC in groundwater under agricultural soil [mg/l]</td>
<td>0.046</td>
<td>-</td>
</tr>
</tbody>
</table>

1) For the estimation of indirect exposure via the environment, the local concentrations calculated for the emission period have to be averaged over the whole year.

The resultant daily doses for the substance are as follows:

- \(\text{DOSE}_{\text{tot}} = 0.036 \text{ mg/kg}_{\text{body weight day}}\) (local scenario)
- \(\text{DOSE}_{\text{tot}} = 3.119 \cdot 10^{-4} \text{ mg/kg}_{\text{body weight day}}\) (regional background concentrations)

The calculated uptake quantities result via the following routes.
### Table 4.2  Route percentages of indirect exposure

<table>
<thead>
<tr>
<th>Uptake route</th>
<th>% of total uptake</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>local</td>
</tr>
<tr>
<td>drinking water</td>
<td>3.61</td>
</tr>
<tr>
<td>fish</td>
<td>0.07</td>
</tr>
<tr>
<td>plant shoot</td>
<td>58.8</td>
</tr>
<tr>
<td>root</td>
<td>0.67</td>
</tr>
<tr>
<td>meat</td>
<td>&lt; 0.01</td>
</tr>
<tr>
<td>milk</td>
<td>0.02</td>
</tr>
<tr>
<td>air</td>
<td>36.8</td>
</tr>
</tbody>
</table>

Drinking water is the most significant route of uptake when using the regional approach. However, the local model indicates consumption of leaf crops and inhalation as main routes for indirect exposure.
5 RESULTS

5.1 ENVIRONMENT

From the intrinsic properties it is expected that propan-1-ol is of low concern for the environment. Therefore, a targeted environmental risk assessment was performed. Using conservative estimates based on worst-case assumptions at the exposure and effects side. The targeted risk assessment results in the following conclusion:

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.

Based on the currently available data, propan-1-ol represents no risk to the environment for the area of production, processing, formulation and use (see Section 3.3).

Although the exposure calculation is based on conservative “worst case” assumptions the calculated environmental concentrations remain clearly under the predicted no effect concentrations.

5.2 HUMAN HEALTH

5.2.1.1 Workers

Conclusion (i) There is a need for further information and/or testing.

For mutagenicity the base set data have to be completed, risk assessment concerning carcinogenicity will be delayed until the mutagenicity data are available.

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

There is a need for limiting the risks of propan-1-ol for several scenarios with short-term and repeated exposures. The most critical exposure route is inhalation, dermal contact being of minor importance. In detail concern is expressed for use of paints, use of cleaning formulations without LEV, short term exposures during use of printing inks.

The toxic effects leading to concern are respiratory depression according to stimulation of the trigeminus nerve, local effects in the airways after repeated exposure and reproductive toxicity concerning fertility as well as developmental toxicity. Risk reduction measures especially for the inhalative exposure situation have to be initiated.

5.2.1.2 Consumers

Conclusion (i) There is a need for further information and/or testing.
Mutagenicity

The minimum requirements in mutagenic testing are not met. An *in vitro* study on chromosome aberration in Chinese hamster cells is currently ongoing.

The producer has to be requested to make available existing studies.

Carcinogenicity

There is no valid carcinogenicity study available. The present data base gives no indication for carcinogenic effects. For performing the risk assessment on carcinogenicity, however, the completed data on mutagenicity have to be taken into account.

5.2.1.3 Humans exposed indirectly via the 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.
REFERENCES


Auty RM and Branch RA (1976). The elimination of ethyl, n-propyl, n-butyl and iso-amyl alcohols by the isolated perfused rat liver. J. Pharmacol. Exp. Ther. 197, 669-674


CHEMSAFE: national database for safety data of the Physikalisch-technische Bundesanstalt Braunschweig, established by expert judgement


Nordman R (1980). Metabolism of some higher alcohols. INSERM (Les Colloques de l’INSERM: Alcohol and the gastrointestinal tract) 95, 187-205.


Petrasol B.V. Gorinchem, HSDB (Hazardous Substances Data Bank), on-line via STN.


Sinclair J, Lambrecht L and Smith EL (1990). Hepatic alcohol dehydrogenase activity in chick hepatocytes towards the major alcohols present in commercial alcoholic beverages: Comparison with activities in rat and human liver. Comp. Biochem. Physiol. 96 (B), 677-682.


# ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADI</td>
<td>Acceptable Daily Intake</td>
</tr>
<tr>
<td>AF</td>
<td>Assessment Factor</td>
</tr>
<tr>
<td>Ann</td>
<td>Annex</td>
</tr>
<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
</tr>
<tr>
<td>ATP</td>
<td>Adaptation to Technical Progress</td>
</tr>
<tr>
<td>AUC</td>
<td>Area Under The Curve</td>
</tr>
<tr>
<td>B</td>
<td>Bioaccumulation</td>
</tr>
<tr>
<td>BBA</td>
<td>Biologische Bundesanstalt für Land- und Forstwirtschaft</td>
</tr>
<tr>
<td>BCF</td>
<td>Bioconcentration Factor</td>
</tr>
<tr>
<td>BMC</td>
<td>Benchmark Concentration</td>
</tr>
<tr>
<td>BMD</td>
<td>Benchmark Dose</td>
</tr>
<tr>
<td>BMF</td>
<td>Biomagnification Factor</td>
</tr>
<tr>
<td>BOD</td>
<td>Biochemical Oxygen Demand</td>
</tr>
<tr>
<td>bw</td>
<td>body weight / Bw, bw</td>
</tr>
<tr>
<td>C</td>
<td>Corrosive (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)</td>
</tr>
<tr>
<td>°C</td>
<td>degrees Celsius (centigrade)</td>
</tr>
<tr>
<td>C50</td>
<td>median immobilisation concentration or median inhibitory concentration 1 / explained by a footnote if necessary</td>
</tr>
<tr>
<td>CA</td>
<td>Chromosome Aberration</td>
</tr>
<tr>
<td>CA</td>
<td>Competent Authority</td>
</tr>
<tr>
<td>CAS</td>
<td>Chemical Abstract Services</td>
</tr>
<tr>
<td>CEC</td>
<td>Commission of the European Communities</td>
</tr>
<tr>
<td>CEN</td>
<td>European Standards Organisation / European Committee for Normalisation</td>
</tr>
<tr>
<td>CEPE</td>
<td>European Committee for Paints and Inks</td>
</tr>
<tr>
<td>CMR</td>
<td>Carcinogenic, Mutagenic and toxic to Reproduction</td>
</tr>
<tr>
<td>CNS</td>
<td>Central Nervous System</td>
</tr>
<tr>
<td>COD</td>
<td>Chemical Oxygen Demand</td>
</tr>
<tr>
<td>CSTEE</td>
<td>Scientific Committee for Toxicity, Ecotoxicity and the Environment (DG SANCO)</td>
</tr>
<tr>
<td>CT50</td>
<td>Clearance Time, elimination or depuration expressed as half-life</td>
</tr>
<tr>
<td>d</td>
<td>Day(s)</td>
</tr>
<tr>
<td>d.wt</td>
<td>dry weight / dw</td>
</tr>
<tr>
<td>dfi</td>
<td>daily food intake</td>
</tr>
<tr>
<td>DG</td>
<td>Directorate General</td>
</tr>
<tr>
<td>DIN</td>
<td>Deutsche Industrie Norm (German norm)</td>
</tr>
<tr>
<td>DNA</td>
<td>DeoxyriboNucleic Acid</td>
</tr>
</tbody>
</table>
DOC Dissolved Organic Carbon

\( DT_{50} \) Degradation half-life or period required for 50 percent dissipation / degradation

\( DT_{50\text{lab}} \) Period required for 50 percent dissipation under laboratory conditions

\( DT_{90} \) Period required for 90 percent dissipation / degradation

\( DT_{90\text{field}} \) Period required for 90 percent dissipation under field conditions

(Define method of estimation)

E Explosive (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)

EASE Estimation and Assessment of Substance Exposure Physico-chemical properties [Model]

\( EbC_{50} \) Effect Concentration measured as 50% reduction in biomass growth in algae tests

EC European Communities

\( EC_{10} \) Effect Concentration measured as 10% effect

\( EC_{50} \) Median Effect Concentration

ECB European Chemicals Bureau

ECETOC European Centre for Ecotoxicology and Toxicology of Chemicals

ECVAM European Centre for the Validation of Alternative Methods

EDC Endocrine Disrupting Chemical

EEC European Economic Communities

EINECS European Inventory of Existing Commercial Chemical Substances

ELINCS European List of New Chemical Substances

EN European Norm

EPA Environmental Protection Agency (USA)

\( ErC_{50} \) Effect Concentration measured as 50% reduction in growth rate in algae tests

ESD Emission Scenario Document

EU European Union

EUSES European Union System for the Evaluation of Substances [Software tool in support of the Technical Guidance Document on risk assessment]

\( F(+) \) (Highly) flammable (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)

FAO Food and Agriculture Organisation of the United Nations

FELS Fish Early Life Stage

foc Organic carbon factor (compartment depending)

G Gram(s)

GLP Good Laboratory Practice

h hour(s)

ha Hectares/h

HEDSET EC/OECD Harmonised Electronic Data Set (for data collection of existing substances)
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>HELCOM</td>
<td>Helsinki Commission - Baltic Marine Environment Protection Commission</td>
</tr>
<tr>
<td>HPLC</td>
<td>High Pressure Liquid Chromatography</td>
</tr>
<tr>
<td>HPVC</td>
<td>High Production Volume Chemical (&gt; 1000 tonnes/annum)</td>
</tr>
<tr>
<td>IARC</td>
<td>International Agency for Research on Cancer</td>
</tr>
<tr>
<td>IC</td>
<td>Industrial Category</td>
</tr>
<tr>
<td>IC50</td>
<td>median Immobilisation Concentration or median Inhibitory Concentration</td>
</tr>
<tr>
<td>ILO</td>
<td>International Labour Organisation</td>
</tr>
<tr>
<td>IPCS</td>
<td>International Programme on Chemical Safety</td>
</tr>
<tr>
<td>ISO</td>
<td>International Organisation for Standardisation</td>
</tr>
<tr>
<td>IUCLID</td>
<td>International Uniform Chemical Information Database (existing substances)</td>
</tr>
<tr>
<td>IUPAC</td>
<td>International Union for Pure and Applied Chemistry</td>
</tr>
<tr>
<td>JEFCFA</td>
<td>Joint FAO/WHO Expert Committee on Food Additives</td>
</tr>
<tr>
<td>JMPR</td>
<td>Joint FAO/WHO Meeting on Pesticide Residues</td>
</tr>
<tr>
<td>kg</td>
<td>kilogram(s)</td>
</tr>
<tr>
<td>Koc</td>
<td>organic carbon normalised distribution coefficient</td>
</tr>
<tr>
<td>Kow</td>
<td>octanol/water partition coefficient</td>
</tr>
<tr>
<td>Kp</td>
<td>solids-water partition coefficient</td>
</tr>
<tr>
<td>kPa</td>
<td>kilo Pascals</td>
</tr>
<tr>
<td>l</td>
<td>litre(s)</td>
</tr>
<tr>
<td>L(E)C₅₀</td>
<td>median Lethal (Effect) Concentration</td>
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<tr>
<td>LAEL</td>
<td>Lowest Adverse Effect Level</td>
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<tr>
<td>LC₅₀</td>
<td>median Lethal Concentration</td>
</tr>
<tr>
<td>LD₅₀</td>
<td>median Lethal Dose</td>
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<tr>
<td>LEV</td>
<td>Local Exhaust Ventilation</td>
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<tr>
<td>LLNA</td>
<td>Local Lymph Node Assay</td>
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<tr>
<td>LOAEL</td>
<td>Lowest Observed Adverse Effect Level</td>
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<td>LOEC</td>
<td>Lowest Observed Effect Concentration</td>
</tr>
<tr>
<td>LOED</td>
<td>Lowest Observed Effect Dose</td>
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<tr>
<td>LOEL</td>
<td>Lowest Observed Effect Level</td>
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<tr>
<td>log</td>
<td>logarithm to the basis 10</td>
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<tr>
<td>m</td>
<td>Meter</td>
</tr>
<tr>
<td>MAC</td>
<td>Maximum Allowable Concentration</td>
</tr>
<tr>
<td>MATC</td>
<td>Maximum Acceptable Toxic Concentration</td>
</tr>
<tr>
<td>MC</td>
<td>Main Category</td>
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<tr>
<td>mg</td>
<td>Milligram(s)</td>
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<tr>
<td>MITI</td>
<td>Ministry of International Trade and Industry, Japan</td>
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<tr>
<td>MOE</td>
<td>Margin of Exposure</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>------------</td>
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<tr>
<td>MOS</td>
<td>Margin of Safety</td>
</tr>
<tr>
<td>MW</td>
<td>Molecular Weight</td>
</tr>
<tr>
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<td>Dangerous for the environment (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)</td>
</tr>
<tr>
<td>NAEL</td>
<td>No Adverse Effect Level</td>
</tr>
<tr>
<td>NOAEL</td>
<td>No Observed Adverse Effect Level</td>
</tr>
<tr>
<td>NOEL</td>
<td>No Observed Effect Level</td>
</tr>
<tr>
<td>NOEC</td>
<td>No Observed Effect Concentration</td>
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<tr>
<td>NTP</td>
<td>National Toxicology Program (USA)</td>
</tr>
<tr>
<td>O</td>
<td>Oxidising (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)</td>
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<tr>
<td>OC</td>
<td>Organic Carbon content</td>
</tr>
<tr>
<td>OECD</td>
<td>Organisation for Economic Cooperation and Development</td>
</tr>
<tr>
<td>OEL</td>
<td>Occupational Exposure Limit</td>
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<tr>
<td>OJ</td>
<td>Official Journal</td>
</tr>
<tr>
<td>OSPAR</td>
<td>Oslo and Paris Convention for the protection of the marine environment of the Northeast Atlantic</td>
</tr>
<tr>
<td>P</td>
<td>Persistent</td>
</tr>
<tr>
<td>PBT</td>
<td>Persistent, Bioaccumulative and Toxic</td>
</tr>
<tr>
<td>PBPK</td>
<td>Physiologically Based Pharmacokinetic modelling</td>
</tr>
<tr>
<td>PBTK</td>
<td>Physiologically Based Toxicokinetic modelling</td>
</tr>
<tr>
<td>PEC</td>
<td>Predicted Environmental Concentration</td>
</tr>
<tr>
<td>pH</td>
<td>logarithm (to the base 10) (of the hydrogen ion concentration {H^+})</td>
</tr>
<tr>
<td>pKa</td>
<td>logarithm (to the base 10) of the acid dissociation constant</td>
</tr>
<tr>
<td>pKb</td>
<td>logarithm (to the base 10) of the base dissociation constant</td>
</tr>
<tr>
<td>PNEC</td>
<td>Predicted No Effect Concentration</td>
</tr>
<tr>
<td>PNEC\textsubscript{water}</td>
<td>Predicted No Effect Concentration in Water</td>
</tr>
<tr>
<td>POP</td>
<td>Persistent Organic Pollutant</td>
</tr>
<tr>
<td>PPE</td>
<td>Personal Protective Equipment</td>
</tr>
<tr>
<td>QSAR</td>
<td>(Quantitative) Structure-Activity Relationship</td>
</tr>
<tr>
<td>R phrases</td>
<td>Risk phrases according to Annex III of Directive 67/548/EEC</td>
</tr>
<tr>
<td>RAR</td>
<td>Risk Assessment Report</td>
</tr>
<tr>
<td>RC</td>
<td>Risk Characterisation</td>
</tr>
<tr>
<td>RfC</td>
<td>Reference Concentration</td>
</tr>
<tr>
<td>RfD</td>
<td>Reference Dose</td>
</tr>
<tr>
<td>RNA</td>
<td>RiboNucleic Acid</td>
</tr>
<tr>
<td>RPE</td>
<td>Respiratory Protective Equipment</td>
</tr>
<tr>
<td>RWC</td>
<td>Reasonable Worst-Case</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>S phrases</td>
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<tr>
<td>SAR</td>
<td>Structure-Activity Relationships</td>
</tr>
<tr>
<td>SBR</td>
<td>Standardised birth ratio</td>
</tr>
<tr>
<td>SCE</td>
<td>Sister Chromatic Exchange</td>
</tr>
<tr>
<td>SDS</td>
<td>Safety Data Sheet</td>
</tr>
<tr>
<td>SETAC</td>
<td>Society of Environmental Toxicology And Chemistry</td>
</tr>
<tr>
<td>SNIF</td>
<td>Summary Notification Interchange Format (new substances)</td>
</tr>
<tr>
<td>SSD</td>
<td>Species Sensitivity Distribution</td>
</tr>
<tr>
<td>STP</td>
<td>Sewage Treatment Plant</td>
</tr>
<tr>
<td>T(+)</td>
<td>(Very) Toxic (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)</td>
</tr>
<tr>
<td>TDI</td>
<td>Tolerable Daily Intake</td>
</tr>
<tr>
<td>TG</td>
<td>Test Guideline</td>
</tr>
<tr>
<td>TGD</td>
<td>Technical Guidance Document</td>
</tr>
<tr>
<td>TNsG</td>
<td>Technical Notes for Guidance (for Biocides)</td>
</tr>
<tr>
<td>TNO</td>
<td>The Netherlands Organisation for Applied Scientific Research</td>
</tr>
<tr>
<td>ThOD</td>
<td>Theoretical Oxygen Demand</td>
</tr>
<tr>
<td>UC</td>
<td>Use Category</td>
</tr>
<tr>
<td>UDS</td>
<td>Unscheduled DNA Synthesis</td>
</tr>
<tr>
<td>UN</td>
<td>United Nations</td>
</tr>
<tr>
<td>UNEP</td>
<td>United Nations Environment Programme</td>
</tr>
<tr>
<td>US EPA</td>
<td>Environmental Protection Agency, USA</td>
</tr>
<tr>
<td>UV</td>
<td>Ultraviolet Region of Spectrum</td>
</tr>
<tr>
<td>UVCB</td>
<td>Unknown or Variable composition, Complex reaction products of Biological material</td>
</tr>
<tr>
<td>µg</td>
<td>microgram(s)</td>
</tr>
<tr>
<td>vB</td>
<td>very Bioaccumulative</td>
</tr>
<tr>
<td>VOC</td>
<td>Volatile Organic Compound</td>
</tr>
<tr>
<td>vP</td>
<td>very Persistent</td>
</tr>
<tr>
<td>vPvB</td>
<td>very Persistent and very Bioaccumulative</td>
</tr>
<tr>
<td>v/v</td>
<td>volume per volume ratio</td>
</tr>
<tr>
<td>w</td>
<td>gram weight</td>
</tr>
<tr>
<td>w/w</td>
<td>weight per weight ratio</td>
</tr>
<tr>
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<td>World Health Organisation</td>
</tr>
<tr>
<td>WWTP</td>
<td>Waste Water Treatment Plant</td>
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<td>Xn</td>
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</tr>
<tr>
<td>Xi</td>
<td>Irritant (Symbols and indications of danger for dangerous substances and preparations according to Annex II of Directive 67/548/EEC)</td>
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</table>
## Appendix A  Distribution and fate

### Propanol CAS Nr. 71-23-8

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting point</td>
<td>MP := 146.65 K</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>VP := 1940 Pa</td>
</tr>
<tr>
<td>Water solubility</td>
<td>SOL := 1000000 mg·l⁻¹</td>
</tr>
<tr>
<td>Part. coefficient octanol/water</td>
<td>LOGP OW := 0.34</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>MOLW := 0.0609 kg·mol⁻¹</td>
</tr>
<tr>
<td>Gas constant</td>
<td>R := 8.3143 Pa·m⁻³·mol⁻¹·K⁻¹</td>
</tr>
<tr>
<td>Temperature</td>
<td>T := 293 K</td>
</tr>
<tr>
<td>Concentration of suspended matter in the river</td>
<td>SUSP water := 15 mg·l⁻¹</td>
</tr>
<tr>
<td>Density of the solid phase</td>
<td>RHO solid := 2500 kg·m⁻³</td>
</tr>
<tr>
<td>Volume fraction water in susp. matter</td>
<td>F_water susp := 0.9</td>
</tr>
<tr>
<td>Volume fraction solids in susp. matter</td>
<td>F_solid susp := 0.1</td>
</tr>
<tr>
<td>Volume fraction of water in sediment</td>
<td>F_water sed := 0.8</td>
</tr>
<tr>
<td>Volume fraction of solids in sediment</td>
<td>F_solid sed := 0.2</td>
</tr>
<tr>
<td>Volume fraction of air in soil</td>
<td>F_air soil := 0.2</td>
</tr>
<tr>
<td>Volume fraction of water in soil</td>
<td>F_water soil := 0.2</td>
</tr>
<tr>
<td>Volume fraction of solids in soil</td>
<td>F_solid soil := 0.6</td>
</tr>
<tr>
<td>Aerobic fraction of the sediment comp.</td>
<td>F_aer sed := 0.1</td>
</tr>
<tr>
<td>Product of CONjunge and SURF</td>
<td>product := 10⁻⁴·Pa</td>
</tr>
</tbody>
</table>

### Distribution air/water: Henry-constant

\[
HENRY := \frac{VP \cdot MOLW}{SOL}
\]

\[
\log \left( \frac{HENRY}{Pa \cdot m³\cdot mol⁻¹} \right) = -0.933
\]

\[
K_{air\_water} := \frac{HENRY}{R \cdot T}
\]

\[
HENRY = 0.117 \cdot Pa \cdot m³\cdot mol⁻¹
\]

\[
K_{air\_water} = 4.785 \cdot 10⁻⁵
\]
solid/water-partition coefficient $K_{p, \text{comp}}$ and total compartment/water-partition coefficient $K_{p, \text{comp, water}}$

$$a := 0.39 \quad (a, b \text{ from TGD, p. 539})$$
$$\text{alcohols}$$
$$b := 0.5$$

$$K_{OC} := 10^{a \cdot \text{LOGP}_{OW} + b \cdot \text{kg}^{-1}}$$

$$K_{OC} = 4.291 \text{kg}^{-1}$$

**Suspended matter**

$$K_{p, \text{susp}} := 0.1 \cdot K_{OC}$$

$$K_{\text{susp, water}} := F_{\text{water, susp}} + F_{\text{solid, susp}} \cdot K_{p, \text{susp}} \cdot RHO_{\text{solid}}$$

$$K_{\text{susp, water}} = 1.007$$

**faktor for the calculation of $C_{\text{local, water}}$:**

$$\text{faktor} := 1 + K_{p, \text{susp}} \cdot S\text{USP}_{\text{water}}$$

$$\text{faktor} = 1$$

**Sediment**

$$K_{p, \text{sed}} := 0.05 \cdot K_{OC}$$

$$K_{\text{sed, water}} := F_{\text{water, sed}} + F_{\text{solid, sed}} \cdot K_{p, \text{sed}} \cdot RHO_{\text{solid}}$$

$$K_{\text{sed, water}} = 0.907$$

**Soil**

$$K_{p, \text{soil}} := 0.02 \cdot K_{OC}$$

$$K_{\text{soil, water}} := F_{\text{air, soil}} \cdot K_{\text{air, water}} + F_{\text{water, soil}} + F_{\text{solid, soil}} \cdot K_{p, \text{soil}} \cdot RHO_{\text{solid}}$$

$$K_{\text{soil, water}} = 0.329$$

**Sludge (activated sludge)**

$$K_{p, \text{sludge}} := 0.37 \cdot K_{OC}$$

$$K_{p, \text{sludge}} = 1.588 \text{kg}^{-1}$$

**Raw sewage**

$$K_{p, \text{sewage}} := 0.30 \cdot K_{OC}$$

$$K_{p, \text{sewage}} = 1.287 \text{kg}^{-1}$$
Elimination in STPs

rate constant in STP: $k = 1 \text{ h}^{-1}$

elimination $P = f(k, \log{\text{pow}}, \log{H}) = 0.678$

fraction directed to surface water $F_{\text{stp\_water}} = 0.322$

biodegradation in different compartments

**surface water**

$kbio_{\text{water}} := 0.047 \text{d}^{-1}$ (cTGD, table 5)

**soil**

$DT_{50\text{bio\_soil}} := 30 \text{d}$ (cTGD, table 6)

$kbio_{\text{soil}} := \frac{\ln(2)}{DT_{50\text{bio\_soil}}} \quad kbio_{\text{soil}} = 0.023 \text{d}^{-1}$

**sediment**

$kbio_{\text{sed}} := \frac{\ln(2)}{DT_{50\text{bio\_soil}}} \frac{Faer_{\text{sed}}}{F_{\text{aer\_product}}} \quad kbio_{\text{sed}} = 2.3 \times 10^{-3} \text{d}^{-1}$

**degradation in surface waters**

$k_{\text{hydr\_water}} := 0 \text{h}^{-1}$

$k_{\text{photo\_water}} := 0 \text{h}^{-1}$

$k_{\text{deg\_water}} := k_{\text{hydr\_water}} + k_{\text{photo\_water}} + kbio_{\text{water}}$

$k_{\text{deg\_water}} = 0.047 \text{d}^{-1}$

**Atmosphere**

calculation of $CON_{\text{nunje}} \ast SURF_{\text{aer}}$ for the OPS-model

$\text{VP} := \exp\left[6.79 \left(\frac{1 - \text{MP}}{285 \text{ K}}\right)\right] \quad \text{VP} := \text{wenn(} \text{MP} > 285 \text{ K, VP}}$ (cTGD, table 7)

$VP = 1.9 \times 10^{3} \text{ Pa}$

$F_{\text{aer\_product}} := \frac{\text{product}}{\text{VP} + \text{product}}

F_{\text{aer\_product}} = 5.155 \times 10^{-8}$

**degradation in the atmosphere**

$k_{\text{deg\_aer}} = 0.00896 \text{ h}^{-1}$ (see AOP-calculation)
Characterization of the chemical

Molecular weight = 60 [g mol⁻¹]

Physical properties

- Solubility: 1.0E+04 [g L⁻¹]
- Vapour pressure: 1.94E+03 [Pa]
- Henry constant (H): 1.17E-01 [Pa m³ mol⁻¹]
- Henry constant (H): 1.17E+03 [kg BOD kg dry wt⁻¹ d⁻¹]
- Henry constant (H): 1.17E+01 [L kg BOD⁻¹]
- Henry constant (H): 1.17E-01 [L kg BOD⁻¹]

Emission scenario

- Temperature: 15 [°C]
- Windspeed: 3 [m s⁻¹]
- Sewage flow: 200 [L person⁻¹ d⁻¹]
- Number inhabitants: 1E+04 [person]
- Sludge loading rate (SRT): 9,2 [d]
- HRT = 6,9 [hr]
- C in solids = 3,3E-01 [mg kg⁻¹]
- C dissolved = 5,0E-01 [mg L⁻¹]

Biodegradation in activated sludge

Method 1: estimated from OECD/EU standardized biodegradability tests (USES 2.0)

Method 2: chemical is biodegradable in activated sludge batch test (draft ISO test)

Method 3: chemical is biodegradable in activated sludge, Monod Kinetics

k biodeg1 = 1 [hr⁻¹]
k biodeg2 = 1 [hr⁻¹]

k biodeg3 = 1 [hr⁻¹]

k biodeg4 = 1 [hr⁻¹]

k biodeg5 = 1 [hr⁻¹]

k biodeg6 = 1 [hr⁻¹]

k biodeg7 = 1 [hr⁻¹]

k biodeg8 = 1 [hr⁻¹]

k biodeg9 = 1 [hr⁻¹]

k biodeg10 = 1 [hr⁻¹]

k biodeg11 = 1 [hr⁻¹]

k biodeg12 = 1 [hr⁻¹]
# EU Risk Assessment Report – Propan-1-ol

## Final Report, 2008

### Output of SimpleTreat 3.0 (debugged version, 7 Feb 97)

#### Report of Propanol

<table>
<thead>
<tr>
<th>Including primary sedimentation</th>
<th>Elimination in the primary settler</th>
<th>Without primary sedimentation</th>
</tr>
</thead>
<tbody>
<tr>
<td>volatilization</td>
<td>0.0%</td>
<td>0.0%</td>
</tr>
<tr>
<td>via primary sludge</td>
<td>0.0%</td>
<td>0.0%</td>
</tr>
<tr>
<td>via surplus sludge</td>
<td>0.0%</td>
<td>0.0%</td>
</tr>
<tr>
<td>total</td>
<td>0.0%</td>
<td>0.0%</td>
</tr>
</tbody>
</table>

#### Elimination in the aerator

| via primary sludge               | 87.3%                               |
| total                            | 87.3%                               |

#### Elimination in the solids liquid separator

| via primary sludge               | 0.0%                               |
| via surplus sludge               | 0.0%                               |
| total                            | 0.0%                               |

**Total elimination from waste water**: 87.4%  
**Total emission via effluent**: 12.6%

#### Summary of distribution

| To air                           | 0.1%                               |
| To water                         | 12.6%                              |
| To air                           | 0.0%                               |
| to water                         | 8.5%                               |

#### Concentrations

| in air                           | 9.79E-09 g m⁻³                     |
| in combined sludge               | 2.62E-01 mg kg⁻¹                   |
| in primary sludge                | 3.28E-01 mg kg⁻¹                   |
| in surplus sludge                | 3.48E-02 mg kg⁻¹                   |
| in effluent (total)              | 4.23E-02 mg l⁻¹                    |
| dissolved                        | 4.23E-02 mg l⁻¹                    |
| associated                       | 1.54E-06 mg l⁻¹                    |
| total                            | 100.0%                             |

#### Operations of the plant equipped with a primary settler

| Sludge loading rate              | 0.15 kg BOD (kg dry wt) d⁻¹       |
| HRT                              | 6.9 d                             |
| Aeration mode                    | surface aeration                  |
| Primary sludge                   | 6.0E+02 kg dry weight d⁻¹         |
| Surplus sludge                   | 3.1E+02 kg dry weight d⁻¹         |
| Total sludge                     | 9.1E+02 kg dry weight d⁻¹         |
| Total wastewater                 | 2.0E+03 m³ d⁻¹                    |

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Appendix B  Clocal\textsubscript{water} Calculation for Processing, Formulation and Use

\textbf{Estimation of Clocal\textsubscript{water} at formulation of household chemicals}
(pharmaceutics, disinfectants, cosmetics and cleaning/washing agents)
status: formulation, IC:5 UC:48

\textbf{chemical : Propanol  CAS-Nr.: 71-23-8}

Total annual tonnage of chemical:
TONNAGE := 1000 tonne \cdot a^{-1}

d := 86400 s

\mu g := 10^{-9} \cdot kg

\textbf{Emission per day:}

E\textsubscript{local water} := \frac{TONNAGE \cdot \text{Fmainsource} \cdot f\text{emission} \cdot T\text{emission}}{1 + \text{Kp} \cdot \text{SUSPwater}}

E\textsubscript{local water} = 4 \mu g \cdot d^{-1}

\textbf{Influent concentration:}

C\textsubscript{local inf} := \frac{E\textsubscript{local water}}{\text{EFFLUENT}_{\text{stp}}}

C\textsubscript{local inf} = 2 \text{mg} \cdot \Gamma^{-1}

\textbf{Effluent concentration:}

C\textsubscript{local eff} := C\textsubscript{local inf} \cdot F\textsubscript{stp water}

C\textsubscript{local eff} = 0.252 \text{mg} \cdot \Gamma^{-1}

\textbf{Concentration in surface water:}

C\textsubscript{local water} := \frac{C\textsubscript{local eff}}{\text{FACTOR} \cdot \text{DILUTION}}

C\textsubscript{local water} = 25.2 \mu g \cdot \Gamma^{-1}

\textbf{Total release for the regional model ( without elimination in STPs ):}

RELEASE := T\text{ONNAGE} \cdot f\text{emission}

RELEASE = 3 \text{tonne} \cdot a^{-1}

\textbf{Annual average local concentration in water:}

C\textsubscript{local water ann} := \frac{C\textsubscript{local water} \cdot T\text{emission}}{365 \cdot d \cdot a^{-1}}

C\textsubscript{local water ann} = 0.021 \text{mg} \cdot \Gamma^{-1}
**Estimation of $C_{\text{local \ water}}$ at formulation of solvent (IC = other)**

- status: TGD,A+B table, IC - 0

**chemical:** Propanol, CAS-Nr.: 71-23-8

Total annual tonnage of chemical:

- Release factor (A 2.1):
- Fraction of main source (B 2.8):
- Waste water flow of wwtp:
- Duration of emission (B 2.8):
- Fraction of emission directed to water: (SimpleTreat; $k$:1$h^{-1}$; $\log Pow$:0.34 ; $\log H$:0.93)

- Dilution factor (TGD):
- Factor $(1+K_p \cdot SUSP_{\text{water}})$:

**Emission per day:**

$$E_{\text{local \ water}} := \frac{\text{TONNAGE} \cdot f_{\text{emission}} \cdot F_{\text{main source}}}{T_{\text{emission}}}$$

$$E_{\text{local \ water}} = 10 \ \text{kg \ d}^{-1}$$

**Influent concentration:**

$$C_{\text{local \ inf}} := \frac{E_{\text{local \ water}}}{C_{\text{Effluent \ stp}}}$$

$$C_{\text{local \ inf}} = 5 \ \text{mg \ l}^{-1}$$

**Effluent concentration:**

$$C_{\text{local \ eff}} := C_{\text{local \ inf}} \cdot F_{\text{stp \ water}}$$

$$C_{\text{local \ eff}} = 0.63 \ \text{mg \ l}^{-1}$$

**Concentration in surface water:**

$$C_{\text{local \ water}} := \frac{C_{\text{local \ eff}}}{\text{FACTOR \ DILUTION}}$$

$$C_{\text{local \ water}} = 63 \ \mu g \ l^{-1}$$

**Total release for the regional model (without elimination in STPs):**

$$\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}}$$

$$\text{RELEASE} = 2 \ \text{tonne} \ \text{a}^{-1}$$

**Annual average local concentration in water:**

$$C_{\text{local \ water \ ann}} := \frac{C_{\text{local \ water}} \cdot T_{\text{emission}}}{365 \ \text{d} \ \text{a}^{-1}}$$

$$C_{\text{local \ water \ ann}} = 34.5 \ \mu g \ l^{-1}$$
Estimation of \( C_{\text{local, water}} \) at formulation of chemicals for paints, laques and varnishes (used as a solvent) 

**status:** TGD,A+B table, IC:14,UC:48

**chemical:** Propanol  **CAS-Nr.: 71-23-8**

Total annual tonnage of chemical: 

Release factor (A 2.1): 

Fraction of main source (B 2.10): 

Waste water flow of wwtp: 

Duration of emission (B 2.10): 

Fraction of emission directed to water: 

(Dilution factor (TGD): 

Factor \((1+K_{p} \cdot \text{SUSP}_{\text{water}})\): 

**Emission per day:** 

\[
E_{\text{local, water}} = \frac{\text{TONNAGE}_{\text{Fmainsource}} \cdot f_{\text{emission}}}{T_{\text{emission}}} \approx 40 \text{ kg d}^{-1}
\]

**Influent concentration:** 

\[
C_{\text{local, inf}} = \frac{E_{\text{local, water}}}{\text{EFFLUENT}_{\text{stp}}} \approx 20 \text{ mg l}^{-1}
\]

**Effluent concentration:** 

\[
C_{\text{local, eff}} = C_{\text{local, inf}} \cdot F_{\text{stp, water}} \approx 2.52 \text{ mg l}^{-1}
\]

**Concentration in surface water:** 

\[
C_{\text{local, water}} = \frac{C_{\text{local, eff}}}{\text{FACTOR \cdot DILUTION}} \approx 252 \mu\text{g l}^{-1}
\]

**Total release for the regional model (without elimination in STPs):** 

\[
\text{RELEASE} = \text{TONNAGE}_{\text{f emission}} \cdot f_{\text{emission}} \approx 12 \text{ tonne a}^{-1}
\]

**Annual average local concentration in water:** 

\[
C_{\text{local, water, ann}} = \frac{C_{\text{local, water}} \cdot T_{\text{emission}}}{365 \cdot \text{d a}^{-1}} \approx 207.1 \mu\text{g l}^{-1}
\]
Calculation of $\text{PEC}_{\text{local}}$ for aquatic compartment during processing of Propanol generic scenario (without specific wwtp)

status: TGD, ESD, IC-3

**chemical:** Propanol

Processing volume:

Emission factor for processing: (TGD, tab. A3.3):

Fraction of the main source - processing (on-site):

Duration of emission for processing; (on-site):

Fraction of emission directed to water:

(Right-Treat, k: 1h-1; logH: -0.93; log$K_{ow}$: 0.34)

River flow rate for processing (TGD):

Factor $(1 + K_p \cdot \text{SUSP}_{\text{water}})$:

Release

\[ \text{RELEASE} = T \cdot f \]

\[ \text{RELEASE} = 95.89 \text{kg d}^{-1} \]

**processing**

Emission per day:

\[ \text{E}_{\text{local, water}} = \frac{T \cdot f}{T_{\text{emission}}} \]

\[ \text{E}_{\text{local, water}} = 116.67 \text{kg d}^{-1} \]

**Concentration in surface water:**

\[ \text{C}_{\text{local, water}} = \frac{\text{E}_{\text{local, water}} \cdot \text{F}_{\text{stp, water}}}{\text{FLOW} \cdot \text{FACTOR}} \]

\[ \text{C}_{\text{local, water}} = 2.84 \text{µg} \cdot \text{L}^{-1} \]
**Estimation of C_{local, water} of chemicals for processing of solvents (IC = 0)**

**status:** TGD,A+B table, IC - 0, MC:3

**chemical:** Propanol  CAS-Nr.: 71-23-8

Total annual tonnage of chemical: TONNAGE := 100 tonne \cdot a^{-1}

Release factor (A 3.16): \( f_{\text{emission}} := 0.01 \)

Fraction of main source (B 3.14): F_{\text{main source}} := 0.8

Waste water flow of wwt: EFFLUENT_{stp} := 2000 m^3 \cdot d^{-1}

Duration of emission (B 3.14): T_{\text{emission}} := 32 d \cdot a^{-1}

Fraction of emission directed to water: F_{\text{stp water}} := 12.6%

Dilution factor (TGD): DILUTION := 10

Factor \((1+K_p \cdot \text{SUSP}_{\text{water}})\): FACTOR := 1

**Emission per day:**

\[
E_{\text{local, water}} := \frac{\text{TONNAGE} \cdot F_{\text{main source}} \cdot f_{\text{emission}}}{T_{\text{emission}}} \quad E_{\text{local, water}} = 25 \text{ kg} \cdot \text{d}^{-1}
\]

**Influent concentration:**

\[
C_{\text{local, inf}} := \frac{E_{\text{local, water}}}{\text{EFFLUENT}_{\text{stp}}} \quad C_{\text{local, inf}} = 12.5 \text{ mg} \cdot \text{l}^{-1}
\]

**Effluent concentration:**

\[
C_{\text{local, eff}} := C_{\text{local, inf}} \cdot F_{\text{stp, water}} \quad C_{\text{local, eff}} = 1.58 \text{ mg} \cdot \text{l}^{-1}
\]

**Concentration in surface water:**

\[
C_{\text{local, water}} := \frac{C_{\text{local, eff}}}{\text{FACTOR} \cdot \text{DILUTION}} \quad C_{\text{local, water}} = 157.5 \text{ µg} \cdot \text{l}^{-1}
\]

**Total release for the regional model (without elimination in STPs):**

\[
\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}} \quad \text{RELEASE} = 1 \text{ tonne} \cdot \text{a}^{-1}
\]

**Annual average local concentration in water:**

\[
C_{\text{local, water, ann}} := \frac{C_{\text{local, water}} \cdot T_{\text{emission}}}{365 \text{ d} \cdot \text{a}^{-1}} \quad C_{\text{local, water, ann}} = 13.8 \text{ µg} \cdot \text{l}^{-1}
\]
Estimation of $C_{\text{local}}$ of chemicals for paints, laques and varnishes at processing in paint shops

status: TGD,A+B table, IC-14 UC:48 $\mu g := 10^{-9}$ kg
d := 86400 s

chemical : Propanol  CAS-Nr.: 71-23-8

Total annual tonnage of chemical:

$\text{TONNAGE} := 600 \text{ tonne \text{ a}^{-1}}$

Release factor (A 3.15):

$f_{\text{emission}} := 0.02$

Fraction of main source (B 3.13):

$F_{\text{main source}} := 0.15$

Waste water flow of WWTP:

$\text{EFFLUENT}_{\text{stp}} := 2000 \text{ m}^3 \text{ d}^{-1}$

Duration of emission (B 3.13):

$T_{\text{emission}} := 300 \text{ d} \cdot \text{a}^{-1}$

Fraction of emission directed to water:

(SimpleTreat; k:1h$^{-1}$; logPow:0.34 ; logH:-0.93)

$F_{\text{stp water}} := 12.6\%$

Dilution factor (TGD):

$\text{DILUTION} := 10$

Factor $(1 + K_p \cdot \text{SUSPwater})$:

$\text{FACTOR} := 1$

**Emission per day:**

$E_{\text{local water}} := \frac{\text{TONNAGE} \cdot F_{\text{main source}} \cdot f_{\text{emission}}}{T_{\text{emission}}}$

$E_{\text{local water}} = 6 \text{ kg d}^{-1}$

**Influent concentration:**

$C_{\text{local inf}} := \frac{E_{\text{local water}}}{\text{EFFLUENT}_{\text{stp}}}$

$C_{\text{local inf}} = 3 \text{ mg l}^{-1}$

**Effluent concentration:**

$C_{\text{local eff}} := C_{\text{local inf}} \cdot F_{\text{stp water}}$

$C_{\text{local eff}} = 0.38 \text{ mg l}^{-1}$

**Concentration in surface water:**

$C_{\text{local water}} := \frac{C_{\text{local eff}}}{\text{FACTOR} \cdot \text{DILUTION}}$

$C_{\text{local water}} = 37.8 \mu g l^{-1}$

**Total release for the regional model (without elimination in STPs):**

$\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}}$

$\text{RELEASE} = 12 \text{ tonne \text{ a}^{-1}}$

**Annual average local concentration in water:**

$C_{\text{local water ann}} := \frac{C_{\text{local water}} \cdot T_{\text{emission}}}{365 \cdot \text{d} \cdot \text{a}^{-1}}$

$C_{\text{local water ann}} = 31.1 \mu g l^{-1}$
Estimation of C_{local\_water} at use of household chemicals
(pharmaceutics, disinfectants, cosmetics and cleaning/washing agents)
status: private use, IC:5 UC:48

**chemical**: Propanol, CAS-Nr.: 71-23-8

- Tonnage of chemical: \( \text{TONNAGE} = 1000000 \text{kg} \cdot \text{a}^{-1} \)
- Fraction of main source (B 4.1): \( F_{\text{mainsource}} = 0.002 \)
- Release factor (A 4.1): \( f_{\text{emission}} = 0.6 \)
- Duration of emission (B 4.1): \( T_{\text{emission}} = 365 \text{d} \cdot \text{a}^{-1} \)
- Fraction of emission directed to water: \( F_{\text{stp\_water}} = 12.6\% \)
- Waste water flow of wastewater (TGD): \( \text{EFFLUENT}_{\text{stp}} = 2000 \text{m}^3 \cdot \text{d}^{-1} \)
- Dilution factor: \( \text{DILUTION} = 10 \)
- Factor \( (1 + K_p \cdot \text{SUSP}_{\text{water}}) \): \( \text{FACTOR} = 1 \)

**Emission per day**:

\[
E_{\text{local\_water}} := \frac{\text{TONNAGE} \cdot F_{\text{mainsource}} \cdot f_{\text{emission}}}{T_{\text{emission}}} = 3.288 \text{kg} \cdot \text{d}^{-1}
\]

**Influent concentration**:

\[
C_{\text{local\_inf}} := \frac{E_{\text{local\_water}}}{\text{EFFLUENT}_{\text{stp}}} = 1.644 \text{mg} \cdot \text{l}^{-1}
\]

**Effluent concentration**:

\[
C_{\text{local\_eff}} := C_{\text{local\_inf}} \cdot F_{\text{stp\_water}} = 207.123 \mu\text{g} \cdot \text{l}^{-1}
\]

**Concentration in receiving water**:

\[
C_{\text{local\_water}} := \frac{C_{\text{local\_eff}}}{\text{DILUTIONFACTOR}} = 20.7 \mu\text{g} \cdot \text{l}^{-1}
\]

**Emission for PEC_{\text{regional}} (without wastewater)**:

\[
\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}} = 600 \text{tonne} \cdot \text{a}^{-1}
\]

**Annual average local concentration in surface water**:

\[
C_{\text{local\_water\_ann}} := C_{\text{local\_water}} = 20.7 \mu\text{g} \cdot \text{l}^{-1}
\]
**Estimation of Clocal\textsubscript{water} of chemicals for paints, laques and varnishes at privat use**

Status: TGD,A+B table, IC-14, UC:48

**chemical**: Propanol, CAS-Nr.: 71-23-8

Total annual tonnage of chemical:

\( \text{TONNAGE} = 600 \text{ tonne \cdot a}^{-1} \)

Release factor (A 4.5):

\( f_{\text{emission}} = 0.04 \)

Fraction of main source (B 4.5):

\( F_{\text{mainsource}} = 0.0004 \)

Waste water flow of wwtp:

\( \text{EFFLUENT}_{\text{stp}} = 2000 \text{ m}^3 \cdot \text{d}^{-1} \)

Duration of emission (B 4.5):

\( T_{\text{emission}} = 300 \text{ d} \cdot \text{a}^{-1} \)

Fraction of emission directed to water:

\( F_{\text{stp water}} = 12.6\% \)

Dilution factor (TGD):

\( \text{DILUTION} = 10 \)

Factor \((1 + Kp \cdot \text{SUSPwater})\):

\( \text{FACTOR} = 1 \)

**Emission per day**:

\[
\text{Elocal water} := \frac{\text{TONNAGE} \cdot F_{\text{mainsource}} \cdot f_{\text{emission}}}{T_{\text{emission}}} = 0.03 \text{ kg} \cdot \text{d}^{-1}
\]

**Influent concentration**:

\[
\text{Clocal \text{inf}} := \frac{\text{Elocal water}}{\text{EFFLUENT}_{\text{stp}}} = 0.016 \text{ mg} \cdot \text{L}^{-1}
\]

**Effluent concentration**:

\[
\text{Clocal \text{eff}} := \text{Clocal \text{inf}} \cdot F_{\text{stp water}} = 2.016 \cdot 10^{-3} \text{ mg} \cdot \text{L}^{-1}
\]

**Concentration in surface water**:

\[
\text{Clocal \text{water}} := \frac{\text{Clocal \text{eff}}}{\text{FACTOR} \cdot \text{DILUTION}} = 0.2 \mu g \cdot \text{L}^{-1}
\]

**Total release for the regional model (without elimination in STPs)**:

\( \text{RELEASE} = \text{TONNAGE} \cdot f_{\text{emission}} = 24 \text{ tonne} \cdot \text{a}^{-1} \)

**Annual average local concentration in water**:

\[
\text{Clocal \text{water ann}} := \frac{\text{Clocal \text{water}} \cdot T_{\text{emission}}}{365 \text{ d} \cdot \text{a}^{-1}} = 0.2 \mu g \cdot \text{L}^{-1}
\]
Appendix C  Clocal\textsubscript{air} calculation for processing, formulation and use
**Atmosphere (OPS-model)**

Calculation of C\textsubscript{local air} and PEC\textsubscript{local air}

**chemical**: Propanol  \hspace{1cm} CAS-Nr.: 71-23-8

**stage of life cycle**: formulation household chemical \hspace{1cm} (pharmaceutics, disinfectants, cosmetics and cleaning/washing agents)

IC: 5  \hspace{1cm} UC: 48  \hspace{1cm} MC: 3

**tonnage for specific scenario:**

- release factor (table A-2.1):
- fraction of main source (table B-2.1):
- days of use per year (table B-2.1):
- release during life cycle to air:

**local emission during episode to air:**

- concentration in air at source
  - strength of 1kg/d
- fraction of the emission to air from STP

**local emission rate to water during emission episode**

**local emission to air from STP during emission episode**

**local concentration in air during emission episode:**

\[ C_{local \text{ air}} := \begin{cases} \text{Estp air} \times C_{std \text{ air}} & \text{if } E_{local \text{ air}} \leq E_{local \text{ air}} \times E_{stp \text{ air}} \times C_{std \text{ air}} \\ C_{local \text{ air}} & \text{otherwise} \end{cases} \]

\[ C_{local \text{ air}} = 9.267 \times 10^{-3} \text{ mg. m}^{-3} \]

\[ C_{local \text{ air}} := \frac{C_{local \text{ air}} \times \text{Temission}}{365 \cdot \text{d} \cdot \text{a}^{-1}} \]

\[ C_{local \text{ air}} = 7.616 \times 10^{-3} \text{ mg. m}^{-3} \]

**PEC regional air**

\[ PEC_{regional \text{ air}} := 9.45 \times 10^{-3} \text{ mg. m}^{-3} \]

**PEC local air**

\[ PEC_{local \text{ air}} := C_{local \text{ air}} + PEC_{regional \text{ air}} \]

\[ PEC_{local \text{ air}} := 7.711 \times 10^{-3} \text{ mg. m}^{-3} \]
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[
\text{DEPstd}_{\text{aer}} := 1 \times 10^{-5} \text{ mg m}^{-2} \text{ d}^{-1} \text{ kg}^{-1} \text{ d}
\]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[
\text{Fass}_{\text{aer}} := 5.155 \times 10^{-8}
\]

deposition flux of gaseous compounds as a function of Henry’s Law coefficient, at a source strength of 1kg/d

\[
\begin{align*}
\text{logH}<2 & \quad 5 \times 10^{-4} \text{ mg m}^{-2} \text{ d}^{-1} \\
-2<\text{logH}<2 & \quad 4 \times 10^{-4} \text{ mg m}^{-2} \text{ d}^{-1} \\
\text{logH}>2 & \quad 3 \times 10^{-4} \text{ mg m}^{-2} \text{ d}^{-1}
\end{align*}
\]

\[
\text{DEPstd}_{\text{gas}} := 4 \times 10^{-4} \text{ mg m}^{-2} \text{ d}^{-1} \text{ kg}^{-1} \text{ d}
\]

total deposition flux during emission episode

\[
\text{DEP}_{\text{total}} := (E_{\text{local air}} + E_{\text{sp air}}) \left[ \text{Fass}_{\text{aer}} \cdot \text{DEPstd}_{\text{aer}} + (1 - \text{Fass}_{\text{aer}}) \cdot \text{DEPstd}_{\text{gas}} \right]
\]

\[
\text{DEP}_{\text{total}} = 0.013 \text{ mg m}^{-2} \text{ d}^{-1}
\]

annual average total deposition flux

\[
\text{DEP}_{\text{total ann}} := \frac{\text{DEP}_{\text{total}} \cdot \text{T}_{\text{emission}}}{365 \text{ d a}^{-1}}
\]

\[
\text{DEP}_{\text{total ann}} = 0.011 \text{ mg m}^{-2} \text{ d}^{-1}
\]
Atmosphere (OPS-model)

Calculation of C_{local\ air} and PEC_{local\ air}

**chemical:** Propanol  \( \text{CAS-Nr.: } 71-23-8 \)

**stage of life cycle:** formulation of solvent not specified

IC:0 UC:48 MC:3

d := 86400s

\( a := 365 \text{ d} \)

\( mg := 1 \cdot 10^{-6} \text{ kg} \)

**tonnage for specific scenario:**

TONNAGE:= 100 tonne \( \text{a}^{-1} \)

release factor (A 2.1):

\( f_{\text{emission}} := 0.025 \)

fraction of main source (table B 2.8):

\( F_{\text{mainsource}} := 1 \)

days of use per year (table B 2.8):

\( T_{\text{emission}} := 200 \text{ d} \text{a}^{-1} \)

release during life cycle to air:

RELEASE:= TONNAGE\( f_{\text{emission}} \)

RELEASE= 2.5 \( \text{tonne} \text{a}^{-1} \)

**local emission during episode to air:**

\[ E_{\text{local\ air}} = \frac{F_{\text{mainsource} \cdot \text{RELEASE}}}{T_{\text{emission}}} \]

\[ E_{\text{local\ air}} = 12.5 \text{ kg d}^{-1} \]

concentration in air at source strength of 1kg/d

\( C_{\text{std\ air}} := 2.78 \cdot 10^{-4} \text{ mg m}^{-3} \cdot \text{kg}^{-1} \cdot \text{d} \)

fraction of the emission to air from STP (App.II)

\( F_{\text{stp\ air}} := 0.1 \% \)

local emission rate to water during emission episode

\( E_{\text{local\ water}} := 10 \text{ kg d}^{-1} \)

local emission to air from STP during emission episode

\( E_{\text{stp\ air}} := F_{\text{stp\ air}} \cdot E_{\text{local\ water}} \)

\( E_{\text{stp\ air}} = 0.01 \text{ kg d}^{-1} \)

**local concentration in air during emission episode:**

\[ C_{\text{local\ air}} := \text{wenn} \left( E_{\text{local\ air}} > E_{\text{stp\ air}} \right) \]

\[ C_{\text{local\ air}} := \frac{E_{\text{local\ air}} - C_{\text{std\ air}}}{E_{\text{stp\ air}} - C_{\text{std\ air}}} \]

\[ C_{\text{local\ air}} = 3.475 \cdot 10^{-3} \text{ mg m}^{-3} \]

annual average concentration in air, 100m from point source

\[ C_{\text{local\ air\ ann}} := C_{\text{local\ air}} \cdot \frac{T_{\text{emission}}}{365 \text{d} \text{a}^{-1}} \]

\[ C_{\text{local\ air\ ann}} = 1.904 \cdot 10^{-3} \text{ mg m}^{-3} \]

**regional concentration in air**

\( \text{PEC}_{\text{regional\ air}} := 9.45 \cdot 10^{-5} \text{ mg m}^{-3} \)

annual average predicted environmental concentration in air

\[ \text{PEC}_{\text{local\ air\ ann}} := C_{\text{local\ air\ ann}} + \text{PEC}_{\text{regional\ air}} \]

\[ \text{PEC}_{\text{local\ air\ ann}} = 1.999 \cdot 10^{-3} \text{ mg m}^{-3} \]
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[
\text{DEP}_{\text{std, aer}} := 1 \times 10^{-2} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d}
\]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[
F_{\text{ass, aer}} := 5.155 \times 10^{-8}
\]

deposition flux of gaseous compounds as a function of Henry’s Law coefficient, at a source strength of 1kg/d

\[
\begin{align*}
\log H < -2 & \quad 5 \times 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \\
-2 < \log H < 2 & \quad 4 \times 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \\
\log H > 2 & \quad 3 \times 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1}
\end{align*}
\]

\[
\text{DEP}_{\text{std, gas}} := 4 \times 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d}
\]

total deposition flux during emission episode

\[
\text{DEP}_{\text{total}} := \left[ \text{Elocal}_{\text{air}} + \text{Estp}_{\text{air}} \right] \left[ F_{\text{ass, aer}} \cdot \text{DEP}_{\text{std, aer}} + (1 - F_{\text{ass, aer}}) \cdot \text{DEP}_{\text{std, gas}} \right]
\]

\[
\text{DEP}_{\text{total}} = 5.004 \times 10^{-3} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1}
\]

annual average total deposition flux

\[
\text{DEP}_{\text{total, ann}} := \text{DEP}_{\text{total}} \cdot \frac{\text{Temission}}{365 \cdot \text{d} \cdot \text{a}^{-1}}
\]

\[
\text{DEP}_{\text{total, ann}} = 2.742 \times 10^{-3} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1}
\]
Atmosphere (OPS-model)

Calculation of Clocal_air and PEC_{local\_air}

**chemical:** Propanol \_CAS-Nr.: 71-23-8

**Stage of life cycle:** formulation of paints
IC:5,6 UC:48 MC:lc

Tonnage for specific scenario:

Release factor (A 2.1):

Fraction of main source (table B 2.10):

Days of use per year (table B 2.10):

Release during life cycle to air:

Local emission during episode to air:

Concentration in air at source strength of 1kg/d

Fraction of the emission to air from STP (App.II)

Local emission rate to water during emission episode

Local emission to air from STP during emission episode

Local concentration in air during emission episode:

Annual average concentration in air, 100m from point source

Regional concentration in air

Annual average predicted environmental concentration in air

\[
d := 86400 \text{s} \\
a := 365 \text{d} \\
mg := 1 \cdot 10^{-6} \text{kg}
\]

\[
f_{\text{emission}} := 0.025 \\
F_{\text{main source}} := 1 \\
T_{\text{emission}} := 300 \cdot \text{d} \cdot \text{a}^{-1} \\
\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}} \\
\text{RELEASE} := 15 \cdot \text{tonne} \cdot \text{a}^{-1}
\]

\[
C_{\text{std\_air}} := 2.78 \cdot 10^{-4} \cdot \text{mg} \cdot \text{m}^{-3} \cdot \text{kg}^{-1} \cdot \text{d} \\
F_{\text{stp\_air}} := 0.1 \% \\
E_{\text{local\_water}} := 40 \cdot \text{kg} \cdot \text{d}^{-1} \\
E_{\text{stp\_air}} := F_{\text{stp\_air}} \cdot E_{\text{local\_water}} \\
E_{\text{stp\_air}} := 0.04 \cdot \text{kg} \cdot \text{d}^{-1}
\]

\[
C_{\text{local\_air\_ann}} := \frac{C_{\text{local\_air}} \cdot T_{\text{emission}}}{365 \cdot \text{d} \cdot \text{a}^{-1}} \\
C_{\text{local\_air\_ann}} := 0.011 \cdot \text{mg} \cdot \text{m}^{-3}
\]

\[
\text{PEC}_{\text{local\_air\_ann}} := C_{\text{local\_air\_ann}} + \text{PEC}_{\text{regional\_air}} \\
\text{PEC}_{\text{local\_air\_ann}} := 0.012 \cdot \text{mg} \cdot \text{m}^{-3}
\]
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[ \text{DEP}_{\text{std\ aer}} := 1 \cdot 10^{-2} \cdot \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d} \]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[ F_{\text{ass\ aer}} := 5.155 \cdot 10^{-8} \]

deposition flux of gaseous compounds as a function of Henry's Law coefficient, at a source strength of 1kg/d

\[
\begin{align*}
\text{DEP}_{\text{std\ gas}} := & \begin{cases} 
5 \cdot 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} & \text{logH} < -2 \\
4 \cdot 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} & -2 < \text{logH} < 2 \\
3 \cdot 10^{-4} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} & \text{logH} > 2 
\end{cases}
\end{align*}
\]

total deposition flux during emission episode

\[ \text{DEP}_{\text{total}} := (\text{E}_{\text{local\ air}} + \text{E}_{\text{sp\ air}}) \left[ F_{\text{ass\ aer}} \cdot \text{DEP}_{\text{std\ aer}} + \left(1 - F_{\text{ass\ aer}}\right) \cdot \text{DEP}_{\text{std\ gas}} \right] \]

\[ \text{DEP}_{\text{total}} = 0.02 \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]

annual average total deposition flux

\[ \text{DEP}_{\text{total\ ann}} := \frac{\text{DEP}_{\text{total}} \cdot \text{T}_{\text{emission}}}{365 \text{d} \cdot \text{a}^{-1}} \]

\[ \text{DEP}_{\text{total\ ann}} = 0.016 \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]
Atmosphere (OPS-model)

**Calculation of \( C_{\text{local air}} \) and \( PEC_{\text{local air}} \)**

**Chemical:** Propanol **CAS-Nr.:** 71-23-8

**Stage of life cycle:** processing  
**Site identification:** generic scenario

Tonnage for scenario:  
Release factor (A 3.3, MC = 3):  
Fraction of main source:  
Days of use per year:  
Release during life cycle to air:  
Local emission during episode to air:

\[
\text{TONNAGE} := 5000 \text{ tonne \cdot a}^{-1}
\]

\[
f_{\text{emission}} := 0.025
\]

\[
F_{\text{main source}} := 1
\]

\[
T_{\text{emission}} := 300 \text{ d \cdot a}^{-1}
\]

\[
\text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}}
\]

\[
\text{RELEASE} = 125 \text{ tonne \cdot a}^{-1}
\]

\[
E_{\text{local air}} := \frac{F_{\text{main source}} \cdot \text{RELEASE}}{T_{\text{emission}}}
\]

\[
E_{\text{local air}} = 416.667 \text{ kg \cdot d}^{-1}
\]

\[
C_{\text{std air}} := 2.78 \cdot 10^{-4} \text{ mg \cdot m}^{-3} \text{ \cdot kg}^{-1} \text{ \cdot d}
\]

\[
F_{\text{stp air}} := 0.1 \%
\]

\[
E_{\text{local water}} := 116.67 \text{ kg \cdot d}^{-1}
\]

\[
E_{\text{stp air}} := F_{\text{stp air}} \cdot E_{\text{local water}}
\]

\[
E_{\text{stp air}} = 0.117 \text{ kg \cdot d}^{-1}
\]

\[
C_{\text{local air}} := \text{wenn } (E_{\text{local air}} > E_{\text{stp air}}, E_{\text{local air}} - C_{\text{std air}}, E_{\text{stp air}} - C_{\text{std air}})
\]

\[
C_{\text{local air}} = 0.116 \text{ mg \cdot m}^{-3}
\]

\[
C_{\text{local air \_ann}} := \frac{C_{\text{local air}} \cdot T_{\text{emission}}}{365 \text{ d} \cdot \text{a}^{-1}}
\]

\[
C_{\text{local air \_ann}} = 0.095 \text{ mg \cdot m}^{-3}
\]

\[
\text{PEC}_{\text{regional air}} := 9.45 \cdot 10^{-5} \text{ mg \cdot m}^{-3}
\]

\[
\text{PEC}_{\text{local air \_ann}} := C_{\text{local air \_ann}} + \text{PEC}_{\text{regional air}}
\]

\[
\text{PEC}_{\text{local air \_ann}} = 0.095 \text{ mg \cdot m}^{-3}
\]
Atmosphere (OPS-model)

Calculation of C_{local \ air} and PEC_{local \ air}

**chemical**: Propanol  \( \text{CAS-Nr.: 71-23-8} \)

**stage of life cycle**: processing of solvent not specified

**IC**: 0  **UC**: 48  **MC**: 3

d := 86400s  \( a := 365 \text{\ d} \)

mg := 1\cdot10^{-6}\text{\ kg}

**tonnage for specific scenario**: TONNAGE := 100\text{tonne} \cdot a^{-1}

**release factor** (A 3.16): \( f_{\text{emission}} := 0.01 \)

**fraction of main source** (table B 3.14): F_{\text{main source}} := 0.8

**days of use per year** (table B 3.14): \( T_{\text{emission}} := 32\text{\ d} \cdot a^{-1} \)

**release during life cycle to air**: \( \text{RELEASE} = \text{TONNAGE} \cdot f_{\text{emission}} \)

**local emission during episode to air**: \( E_{\text{local air}} = \frac{F_{\text{main source}} \cdot \text{RELEASE}}{T_{\text{emission}}} \)

\[ E_{\text{local air}} = 25\text{\ kg} \cdot \text{d}^{-1} \]

**concentration in air at source strength of 1kg/d**: \( C_{\text{std air}} := 2.78\cdot10^{-4}\text{\ mg} \cdot \text{m}^{-3} \cdot \text{kg}^{-1} \cdot \text{d} \)

**fraction of the emission to air from STP (App.II)**: \( F_{\text{stp air}} := 0.1\% \)

**local emission rate to water during emission episode**: \( E_{\text{local water}} := 25\text{\ kg} \cdot \text{d}^{-1} \)

**local emission to air from STP during emission episode**: \( E_{\text{stp air}} := F_{\text{stp air}} \cdot E_{\text{local water}} \)

\[ E_{\text{stp air}} = 0.025\text{\ kg} \cdot \text{d}^{-1} \]

**local concentration in air during emission episode**: \( C_{\text{local air}} := \text{wenn} \left( E_{\text{local air}} > E_{\text{stp air}} \cdot C_{\text{std air}} \right) \)

\[ C_{\text{local air}} = 6.95 \cdot 10^{-3}\text{\ mg} \cdot \text{m}^{-3} \]

**annual average concentration in air, 100m from point source**: \( C_{\text{local air \ ann}} := C_{\text{local air}} \cdot \frac{T_{\text{emission}}}{365\text{\ d} \cdot a^{-1}} \)

\[ C_{\text{local air \ ann}} = 6.09 \cdot 10^{-4}\text{\ mg} \cdot \text{m}^{-3} \]

**regional concentration in air**: \( PEC_{\text{regional air}} := 9.45 \cdot 10^{-5}\text{\ mg} \cdot \text{m}^{-3} \)

**annual average predicted environmental concentration in air**: \( PEC_{\text{local air \ ann}} := C_{\text{local air \ ann}} + PEC_{\text{regional air}} \)

\[ PEC_{\text{local air \ ann}} = 7.03 \cdot 10^{-4}\text{\ mg} \cdot \text{m}^{-3} \]
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[ \text{DEP}_{\text{std aer}} = 1 \cdot 10^{-2} \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d} \]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[ F_{\text{ass aer}} = 5.155 \times 10^{-8} \]

deposition flux of gaseous compounds as a function of Henry’s Law coefficient, at a source strength of 1kg/d

\[
\begin{align*}
\log H &< 2 & 5 \times 10^{-4} \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \\
-2 &< \log H &< 2 & 4 \times 10^{-4} \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \\
\log H &> 2 & 3 \times 10^{-4} \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1}
\end{align*}
\]

\[ \text{DEP}_{\text{std gas}} = 4 \times 10^{-4} \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d} \]

total deposition flux during emission episode

\[
\text{DEP}_{\text{total}} := (E_{\text{local air}} + E_{\text{stp air}}) \left[ F_{\text{ass aer}} \cdot \text{DEP}_{\text{std aer}} + (1 - F_{\text{ass aer}}) \cdot \text{DEP}_{\text{std gas}} \right]
\]

\[ \text{DEP}_{\text{total}} = 0.01 \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]

annual average total deposition flux

\[
\text{DEP}_{\text{total ann}} := \frac{\text{DEP}_{\text{total}} \cdot \text{T}_{\text{emission}}}{365 \cdot \text{d} \cdot \text{a}^{-1}}
\]

\[ \text{DEP}_{\text{total ann}} = 8.776 \times 10^{-4} \text{ mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]
Atmosphere (OPS-model)

Calculation of \( \text{C}_{\text{local air}} \) and \( \text{PEC}_{\text{local air}} \)

**chemical:** Propanol \( \text{CAS-Nr.: 71-23-8} \)

**stage of life cycle:** processing of paints in paint shops

### tonnage for specific scenario:

\[ \text{TONNAGE} := 600 \text{tonne} \cdot \text{a}^{-1} \]

### release factor (table A 3.15):

\[ f_{\text{emission}} := 0.9 \]

### fraction of main source (table B 3.13):

\[ F_{\text{mainsource}} := 0.15 \]

### days of use per year (table B 3.13):

\[ T_{\text{emission}} := 300 \text{d} \cdot \text{a}^{-1} \]

### release during life cycle to air:

\[ \text{RELEASE} := \text{TONNAGE} \cdot f_{\text{emission}} \]

\[ \text{RELEASE} = 540 \text{tonne} \cdot \text{a}^{-1} \]

### local emission during episode to air:

\[ \text{E}_{\text{local air}} := \frac{F_{\text{mainsource}} \cdot \text{RELEASE}}{T_{\text{emission}}} \]

\[ \text{E}_{\text{local air}} = 270 \text{kg} \cdot \text{d}^{-1} \]

### concentration in air at source strength of 1kg/d

\[ C_{\text{std air}} := 2.78 \cdot 10^{-4} \text{mg} \cdot \text{m}^{-3} \cdot \text{kg}^{-1} \cdot \text{d} \]

### fraction of the emission to air from STP (App.II)

\[ F_{\text{stp air}} := 0.1\% \]

### local emission rate to water during emission episode

\[ \text{E}_{\text{local water}} := 6 \text{kg} \cdot \text{d}^{-1} \]

### local emission to air from STP during emission episode

\[ \text{Est}_{\text{p air}} := F_{\text{stp air}} \cdot \text{E}_{\text{local water}} \]

\[ \text{Est}_{\text{p air}} = 6 \cdot 10^{-3} \text{kg} \cdot \text{d}^{-1} \]

### local concentration in air during emission episode:

\[ \text{C}_{\text{local air}} := \begin{cases} \text{E}_{\text{local air}} > \text{Est}_{\text{p air}} & \text{E}_{\text{local air}} \cdot C_{\text{std air}} > \text{Est}_{\text{p air}} \cdot C_{\text{std air}} \\ \text{C}_{\text{local air}} := 0.075 \text{mg} \cdot \text{m}^{-3} \end{cases} \]

### annual average concentration in air, 100m from point source

\[ \text{C}_{\text{local air \_ann}} := \frac{\text{C}_{\text{local air}} \cdot T_{\text{emission}}}{365 \cdot \text{d} \cdot \text{a}^{-1}} \]

\[ \text{C}_{\text{local air \_ann}} = 0.062 \text{mg} \cdot \text{m}^{-3} \]

### regional concentration in air

\[ \text{PEC}_{\text{regional air}} := 9.45 \cdot 10^{-5} \text{mg} \cdot \text{m}^{-3} \]

### annual average predicted environmental concentration in air

\[ \text{PEC}_{\text{local air \_ann}} := \text{C}_{\text{local air \_ann}} + \text{PEC}_{\text{regional air}} \]

\[ \text{PEC}_{\text{local air \_ann}} = 0.062 \text{mg} \cdot \text{m}^{-3} \]
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[ \text{DEP}_{\text{std aer}} := 1 \cdot 10^{-2} \cdot \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d} \]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[ \text{Fass aer} := 5.155 \cdot 10^{-8} \]

deposition flux of gaseous compounds as a function of Henry’s Law coefficient, at a source strength of 1kg/d

\[ \log H < -2 \quad 5 \cdot 10^{-4} \quad \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]
\[ -2 < \log H < 2 \quad 4 \cdot 10^{-4} \quad \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]
\[ \log H > 2 \quad 3 \cdot 10^{-4} \quad \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]

DEP\_{\text{std gas}} := 4 \cdot 10^{-4} \cdot \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \cdot \text{kg}^{-1} \cdot \text{d}

total deposition flux during emission episode

\[ \text{DEP}_{\text{total}} := \left( \text{Elocal air} + \text{Estp air} \right) \left[ \text{Fass aer} \cdot \text{DEP}_{\text{std aer}} + \left( 1 - \text{Fass aer} \right) \cdot \text{DEP}_{\text{std gas}} \right] \]

\[ \text{DEP}_{\text{total}} = 0.108 \cdot \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]

annual average total deposition flux

\[ \text{DEP}_{\text{total ann}} := \frac{\text{DEP}_{\text{total}} \cdot \text{Temission}}{365 \cdot \text{d} \cdot \text{a}^{-1}} \]

\[ \text{DEP}_{\text{total ann}} = 0.089 \cdot \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \]
Atmosphere (OPS-model)
Calculation of $C_{local\ air}$ and PEC $local\ air$

**chemical**: Propanol, CAS-Nr.: 71-23-8

**stage of life cycle**: privat use of paints

- **tonnage for specific scenario**: $TONNAGE := 600\ \text{tonne} \cdot \text{a}^{-1}$
- **release factor (table A 4.5)**: $f_{\text{emission}} := 0.95$
- **fraction of main source (table B 4.5)**: $F_{\text{mainsource}} := 0.0004$
- **days of use per year (table B 4.5)**: $T_{\text{emission}} := 300\ \text{d} \cdot \text{a}^{-1}$
- **release during life cycle to air**: $\text{RELEASE} := TONNAGE \cdot f_{\text{emission}}$
- **local emission during episode to air**: $E_{local\ air} := \frac{F_{\text{mainsource}} \cdot \text{RELEASE}}{T_{\text{emission}}}$

- **concentration in air at source strength of 1kg/d**: $C_{std\ air} := 2.78 \times 10^{-4}\ \text{mg} \cdot \text{m}^{-3} \cdot \text{kg}^{-1} \cdot \text{d}$

- **fraction of the emission to air from STP (App.II)**
- **local emission rate to water during emission episode**: $E_{local\ water} := 0.03\ \text{kg} \cdot \text{d}^{-1}$

- **local emission to air from STP during emission episode**: $E_{stp\ air} := F_{stp\ air} \cdot E_{local\ water}$

- **local concentration in air during emission episode**: $C_{local\ air} := \begin{cases} E_{local\ air} > E_{stp\ air} & E_{local\ air} - C_{std\ air} > E_{stp\ air} - C_{std\ air} \\ E_{local\ air} \leq E_{stp\ air} & E_{stp\ air} \cdot C_{std\ air} \end{cases}$

- **annual average concentration in air, 100m from point source**: $C_{local\ air\ ann} := \frac{C_{local\ air} \cdot T_{\text{emission}}}{365\ \text{d} \cdot \text{a}^{-1}}$

- **regional concentration in air**: $PE_{\text{Regional\ air}} := 9.45 \times 10^{-5}\ \text{mg} \cdot \text{m}^{-3}$

- **annual average predicted environmental concentration in air**: $PE_{local\ air\ ann} := C_{local\ air\ ann} + PE_{\text{Regional\ air}}$

- **PEC local air annual**: $PE_{local\ air\ ann} := 2.68 \times 10^{-4}\ \text{mg} \cdot \text{m}^{-3}$
Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

\[ \text{DEP}_{\text{std aer}} := 1 \times 10^{-2} \text{mg m}^{-2} \text{d}^{-1} \text{kg}^{-1} \text{d} \]

fraction of the chemical bound to aerosol (see: Distribution and Fate)

\[ \text{Fass}_{\text{aer}} := 5.155 \times 10^{-8} \]

deposition flux of gaseous compounds as a function of Henry’s Law coefficient, at a source strength of 1kg/d

\[
\begin{align*}
\log H < -2 & \quad 5 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1} \\
-2 < \log H < 2 & \quad 4 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1} \\
\log H > 2 & \quad 3 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1}
\end{align*}
\]

\[ \text{DEP}_{\text{std gas}} := 4 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1} \text{kg}^{-1} \text{d} \]

total deposition flux during emission episode

\[
\text{DEP}_{\text{total}} := (\text{E}_{\text{local air}} + \text{Est}_{\text{air}}) \left[ \text{Fass}_{\text{aer}} \cdot \text{DEP}_{\text{std aer}} + \left(1 - \text{Fass}_{\text{aer}}\right) \cdot \text{DEP}_{\text{std gas}} \right]
\]

\[ \text{DEP}_{\text{total}} = 3.04 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1} \]

annual average total deposition flux

\[
\text{DEP}_{\text{total ann}} := \frac{\text{DEP}_{\text{total}} \cdot \text{Temission}}{365 \text{ d } \cdot \text{a}^{-1}}
\]

\[ \text{DEP}_{\text{total ann}} = 2.49873 \times 10^{-4} \text{mg m}^{-2} \text{d}^{-1} \]
Appendix D  Exposure of soil

Exposure of Soil

**chemical**: Propanol  CAS-Nr.:71-23-8

**formulation of household chemicals**

annual average total deposition flux:

soil-water partitioning coefficient:

concentration in dry sewage sludge:

air-water partitioning coefficient:

rate constant for for removal from top soil:

PECregional:

**Defaults:**

mixing depth of soil:

bulk density of soil:

average time for exposure:

partial mass transfer coefficient at air-side of the air-soil interface:

partial mass transfer coefficient at soilair-side of the air-soil interface:

partial mass transfer coefficient at soilwater-side of the air-soil interface:

fraction of rain water that infiltrates into soil:

rate of wet precipitation:

\[
\text{DEPTH}_\text{soil} := \begin{align*}
0.2 \text{ m} \\
0.2 \text{ m} \\
0.1 \text{ m}
\end{align*}
\]

\[
\text{RHO}_\text{soil} := 1700 \text{ kg m}^{-3}
\]

\[
T_i := \begin{align*}
30 \text{ d} \\
180 \text{ d} \\
180 \text{ d}
\end{align*}
\]

\[
\text{kasl} _\text{air} := 120 \text{ m d}^{-1}
\]

\[
\text{kasl} _\text{soilair} := 0.48 \text{ m d}^{-1}
\]

\[
\text{kasl} _\text{soilwater} := 4.8 \times 10^{-5} \text{ m d}^{-1}
\]

\[
\text{Finf} _\text{soil} := 0.25
\]

\[
\text{RAINrate} := 1.92 \times 10^{-3} \text{ m d}^{-1}
\]
dry sludge application rate: \( \text{APPL}_{\text{sludge}_i} := \)

\[
\begin{align*}
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.1 \text{ kg m}^{-2} \text{ a}^{-1}
\end{align*}
\]

Calculation:

aerial deposition flux per kg of soil:

\[
D_{\text{air}_i} := \frac{\text{DEP}_{\text{total} \_\text{ann}}}{\text{DEPTH}_{\text{soil}_i} \cdot \text{RHO}_{\text{soil}}}
\]

rate constant for volatilisation from soil:

\[
k_{\text{volat}_i} := \left( \frac{1}{\text{kasl}_{\text{air}} \cdot K_{\text{air} \_\text{water}}} + \frac{1}{\text{kasl}_{\text{soil} \_\text{air}} \cdot K_{\text{air} \_\text{water}} + \text{kasl}_{\text{soil} \_\text{water}}} \right) \cdot K_{\text{soil} \_\text{water}} \cdot \text{DEPTH}_{\text{soil}_i}^{-1}
\]

rate constant for leaching from soil layer:

\[
k_{\text{leach}_i} := \frac{\text{Finf}_{\text{soil}} \cdot \text{RAINrate}}{\text{K}_{\text{soil} \_\text{water}} \cdot \text{DEPTH}_{\text{soil}_i}}
\]

removal from top soil:

\[
k_i := k_{\text{volat}_i} + k_{\text{leach}_i} + k_{\text{bio \_soil}}
\]

concentration in soil

concentration in soil due to 10 years of continuous deposition:

\[
C_{\text{dep}_{\text{soil} \_10_{i}}} := \frac{D_{\text{air}_i}}{k_i} \cdot \left( 1 - \exp(-365 \cdot 10 \cdot k_i) \right)
\]

concentration just after the first year of sludge application:

\[
C_{\text{sludge}_{\text{soil} \_1}_{i}} := \frac{C_{\text{sludge}} \cdot \text{APPL}_{\text{sludge}_i} \cdot \text{a}}{\text{DEPTH}_{\text{soil}_i} \cdot \text{RHO}_{\text{soil}}}
\]

initial concentration in soil after 10 applications of sludge:

\[
C_{\text{sludge}_{\text{soil} \_10_{i}}} := C_{\text{sludge}_{\text{soil} \_1}_{i}} \left[ 1 + \sum_{n=1}^{9} \left( \exp(-365 \cdot k_i) \right)^n \right]
\]
sum of the concentrations due to both processes:

\[ C_{soil\_10\_i} := C_{dep\_soil\_10\_i} + C_{sludge\_soil\_10\_i} \]

average concentration in soil over \( T \) days:

\[
C_{local\_soil\_i} = \frac{D_{air\_i}}{k_i} + \frac{1}{k_i \cdot T_i} \left( C_{soil\_10\_i} - \frac{D_{air\_i}}{k_i} \cdot \left(1 - \exp(-k_i \cdot T_i)\right)\right)
\]

**PEC_{local\_soil\_i} := C_{local\_soil\_i} + PEC_{regional\_natural\_soil}**

<table>
<thead>
<tr>
<th>Local soil</th>
<th>PEC_{local_soil_i}</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>ppm</td>
</tr>
<tr>
<td>1.032 \times 10^{-3}</td>
<td>1.557 \times 10^{-3}</td>
</tr>
<tr>
<td>1.032 \times 10^{-3}</td>
<td>1.557 \times 10^{-3}</td>
</tr>
<tr>
<td>1.629 \times 10^{-3}</td>
<td>2.154 \times 10^{-3}</td>
</tr>
</tbody>
</table>

**Indicating persistency of the substance in soil**

initial concentration after 10 years:

\[ C_{soil\_10\_i} \]

<table>
<thead>
<tr>
<th>ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.032 \times 10^{-3}</td>
</tr>
<tr>
<td>1.032 \times 10^{-3}</td>
</tr>
<tr>
<td>1.629 \times 10^{-3}</td>
</tr>
</tbody>
</table>

initial concentration in steady-state situation:

\[ C_{soil\_ss\_i} := \frac{D_{air\_i}}{k_i} + C_{sludge\_soil\_1\_i} \cdot \frac{1}{1 - Facc_i} \]

<table>
<thead>
<tr>
<th>ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.032 \times 10^{-3}</td>
</tr>
<tr>
<td>1.032 \times 10^{-3}</td>
</tr>
<tr>
<td>1.629 \times 10^{-3}</td>
</tr>
</tbody>
</table>

fraction of steady-state in soil achieved:

\[ Fst\_st\_i := \frac{C_{soil\_ss\_i}}{C_{soil\_10\_i}} \]

<table>
<thead>
<tr>
<th>Fst_st_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>1</td>
</tr>
</tbody>
</table>
concentration in pore water

\[
C_{\text{local soil porew}} := \frac{C_{\text{local RHO soil}}}{K_{\text{soil water}}}
\]

\[
C_{\text{local soil porew}} = 5.33056 \times 10^{-3}
\]

\[
C_{\text{local agr soil porew}} = 5.33056 \times 10^{-3}
\]

\[
C_{\text{local grassland porew}} = 8.41703 \times 10^{-3}
\]

\[
P_{\text{PEClocal soil porew}} := \frac{P_{\text{PEClocal RHO soil}}}{K_{\text{soil water}}}
\]

\[
P_{\text{PEClocal soil porew}} = 8.04332 \times 10^{-3}
\]

\[
P_{\text{PEClocal agr soil porew}} = 8.04332 \times 10^{-3}
\]

\[
P_{\text{PEClocal grassland porew}} = 0.01113
\]

concentration in ground water

\[
P_{\text{PEClocal grw}} = P_{\text{PEClocal agr soil porew}}
\]
Exposure of Soil

**chemical**: Propanol  CAS-Nr.:71-23-8
Formulation of solvents (not specified)

annual average total deposition flux:

soil-water partitioning coefficient:

concentration in dry sewage sludge:

air-water partitioning coefficient:

rate constant for for removal from top soil:

PECregional:

**Defaults:**

mixing depth of soil:

bulk density of soil:

average time for exposure:

partial mass transfer coefficient at air-side of the air-soil interface:

partial mass transfer coefficient at soilair-side of the air-soil interface:

partial mass transfer coefficient at soilwater-side of the air-soil interface:

fraction of rain water that infiltrates into soil:

rate of wet precipitation:

\[
\begin{align*}
\text{DEPtotal}_{\text{ann}} & := 0.00274 \, \text{mg} \cdot \text{m}^{-2} \cdot \text{d}^{-1} \\
K_{\text{soil-water}} & := 0.329 \\
C_{\text{sludge}} & := 0 \, \text{mg} \cdot \text{kg}^{-1} \\
K_{\text{air-water}} & := 0.000048 \\
k_{\text{bio soil}} & := 0.023 \, \text{d}^{-1} \\
\end{align*}
\]

\[
\begin{align*}
\text{PECregional}_{\text{natural soil}} & := 5.25 \times 10^{-4} \, \text{mg} \cdot \text{kg}^{-1} \\
\end{align*}
\]

\[
\begin{align*}
\text{DEPTHsoil} & := \\
0.2 \, \text{m} & \\
0.2 \, \text{m} & \\
0.1 \, \text{m} & \\
\end{align*}
\]

\[
\begin{align*}
\text{RHOsoil} & := 1700 \, \text{kg} \cdot \text{m}^{-3} \\
T_i & := \\
30 \, \text{d} & \\
180 \, \text{d} & \\
180 \, \text{d} & \\
\end{align*}
\]

\[
\begin{align*}
k_{\text{as leaf}} & := 120 \, \text{m} \cdot \text{d}^{-1} \\
k_{\text{soil-air}} & := 0.48 \, \text{m} \cdot \text{d}^{-1} \\
k_{\text{soil-water}} & := 4.8 \times 10^{-5} \, \text{m} \cdot \text{d}^{-1} \\
k_{\text{bio soil}} & := 0.25 \\
\text{RAINrate} & := 1.92 \times 10^{-3} \, \text{m} \cdot \text{d}^{-1} \\
\end{align*}
\]
dry sludge application rate:

\[
\text{APPL}_{\text{sludge}} := \begin{cases} 
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.1 \text{ kg m}^{-2} \text{ a}^{-1} 
\end{cases}
\]

**Calculation:**

aerial deposition flux per kg of soil:

\[
D_{\text{air}} := \frac{\text{DEP}_{\text{total ann}}}{\text{DEPTH}_i \cdot \text{RHO}_i}
\]

rate constant for valatilisation from soil:

\[
k_{\text{volat}} := \left[ \frac{1}{K_{\text{air}} \cdot K_{\text{air-water}}} + \frac{1}{K_{\text{soil-air}} \cdot K_{\text{air-water}} + K_{\text{soil-water}}} \right] \cdot K_{\text{soil-water}} \cdot \text{DEPTH}_i
\]

rate constant for leaching from soil layer:

\[
k_{\text{leach}} := \frac{\text{Finf}_i \cdot \text{RAINrate}}{K_{\text{soil-water}} \cdot \text{DEPTH}_i}
\]

removal from top soil:

\[
k_{i} := k_{\text{volat}} + k_{\text{leach}} + k_{\text{bio soil}}
\]

**concentration in soil**

concentration in soil due to 10 years of continuous deposition:

\[
C_{\text{dep soil \_10}} := \frac{D_{\text{air}}}{k_{i}} \cdot \left( 1 - \exp(-365 \cdot 10 \cdot k_{i}) \right)
\]

concentration just after the first year of sludge application:

\[
C_{\text{sludge soil \_1}} := \frac{C_{\text{sludge}} \cdot \text{APPL}_{\text{sludge}}}{\text{DEPTH}_i \cdot \text{RHO}_i}
\]

initial concentration in soil after 10 applications of sludge:

\[
C_{\text{sludge soil \_10}} := C_{\text{sludge soil \_1}} \cdot \left[ 1 + \sum_{n=1}^{9} \exp(-365 \cdot k_{i}^{n}) \right]
\]
sum of the concentrations due to both processes:
\[ C_{\text{soil}_10i} := C_{\text{dep soil}_10i} + C_{\text{sludge soil}_10i} \]

average concentration in soil over T days:
\[ C_{\text{local soil}_i} := \frac{D_{\text{air}_i}}{k_i} + \frac{1}{k_i \cdot T} \left( C_{\text{soil}_10i} - \frac{D_{\text{air}_i}}{k_i} \cdot (1 - \exp(-k_i \cdot T)) \right) \]

\[ \text{PEC}_{\text{local soil}_i} := C_{\text{local soil}_i} + \text{PEC}_{\text{regional natural soil}} \]

<table>
<thead>
<tr>
<th>C_{\text{local soil}_i}</th>
<th>\text{ppm}</th>
<th>\text{PEC}_{\text{local soil}_i}</th>
<th>\text{ppm}</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2.57 \times 10^{-4})</td>
<td>(7.82 \times 10^{-4})</td>
<td>(2.57 \times 10^{-4})</td>
<td>(7.82 \times 10^{-4})</td>
</tr>
</tbody>
</table>

**Indicating persistency of the substance in soil**

initial concentration after 10 years:
\[ C_{\text{soil}_10i} \text{ ppm} \]

| \(2.57 \times 10^{-4}\) | \(2.57 \times 10^{-4}\) | \(4.058 \times 10^{-4}\) |

initial concentration in steady-state situation:
\[ C_{\text{soil}_\text{ss}_i} := \frac{D_{\text{air}_i}}{k_i} + C_{\text{sludge soil}_1i} \cdot \frac{1}{1 - F\text{acc}_i} \]

\[ C_{\text{soil}_\text{ss}_i} \text{ ppm} \]

| \(2.57 \times 10^{-4}\) | \(2.57 \times 10^{-4}\) | \(4.058 \times 10^{-4}\) |

fraction of steady-state in soil achieved:
\[ F_{\text{st}_1} := \frac{C_{\text{soil}_10i}}{C_{\text{soil}_\text{ss}_i}} \]

| \(\frac{1}{1}\) | \(\frac{1}{1}\) | \(\frac{1}{1}\) |
**concentration in pore water**

\[ C_{\text{local soil_porew}} = \frac{C_{\text{local soil_porew}} - \text{RHO}_{\text{soil}}}{K_{\text{soil_water}}} \]

\[ PEC_{\text{local soil_porew}} = \frac{PEC_{\text{local soil_porew}} - \text{RHO}_{\text{soil}}}{K_{\text{soil_water}}} \]

**concentration in ground water**

\[ PEC_{\text{local grw}} = PEC_{\text{local agr_soil_porew}} \]
Exposure of Soil

chemical: Propanol  CAS-Nr.:71-23-8
processing generic

annual average total deposition flux:
soil-water partitioning coefficient:
concentration in dry sewage sludge:
air-water partitioning coefficient:
rate constant for for removal from top soil:
PECregional:

Defaults:
mixing depth of soil:
bulk density of soil:
average time for exposure:

partial mass transfer coefficient at air-side of the air-soil interface:
partial mass transfer coefficient at soilair-side of the air-soil interface:
partial mass transfer coefficient at soilwater-side of the air-soil interface:
fraction of rain water that infiltrates into soil:
rate of wet precipitation:

DEPtotal\text{ann} := 0.137 \text{mg}\cdot\text{m}^{-2}\cdot\text{d}^{-1}
K_{\text{soil\_water}} := 0.329
C_{\text{sludge}} := 0.0\text{mg}\cdot\text{kg}^{-1}
K_{\text{air\_water}} := 0.000048
k_{\text{bio\_soil}} := 0.023 \text{d}^{-1}

PEC_{\text{regional\_natural\_soil}} := 5.25 \times 10^{-4} \text{mg}\cdot\text{kg}^{-1}

DEPTH_{\text{soil}} :=
0.2 m
0.2 m
0.1 m

RHO_{\text{soil}} := 1700 \text{kg}\cdot\text{m}^{-3}
T_i :=
30\text{d}
180\text{d}
180\text{d}

k_{\text{asl\_air}} := 120 \text{m}\cdot\text{d}^{-1}

k_{\text{asl\_soil\_air}} := 0.48 \text{m}\cdot\text{d}^{-1}

k_{\text{asl\_soil\_water}} := 4.8 \times 10^{-5} \text{m}\cdot\text{d}^{-1}

Finf_{\text{soil}} := 0.25

RAINrate := 1.92 \times 10^{-3} \text{m}\cdot\text{d}^{-1}

\begin{align*}
d &:= 86400 \text{s} \\
ppt &:= \text{mg}\cdot\text{kg}^{-1} \\
a &:= 365 \text{d} \\
i &:= 1.3 \\
C_{\text{sludge}} &:= 0.0\text{mg}\cdot\text{kg}^{-1} \\
k_{\text{bio\_soil}} &:= 0.023 \text{d}^{-1}
\end{align*}
dry sludge application rate: 

\[
\text{APPL}_{\text{sludge}} := \\
\begin{array}{c}
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\
0.1 \text{ kg m}^{-2} \text{ a}^{-1}
\end{array}
\]

**Calculation:**

aerial deposition flux per kg of soil:

\[
D_{\text{air}} := \frac{\text{DEP}_{\text{total ann}}}{\text{DEPTH}_{\text{soil}} \cdot \text{RHO}_{\text{soil}}}
\]

rate constant for volatilisation from soil:

\[
k_{\text{volat}} := \left[ \frac{1}{\text{k}_{\text{soil}} \cdot \text{K}_{\text{air-water}}} + \frac{1}{\text{k}_{\text{soil-air}} \cdot \text{K}_{\text{air-water}} + \text{k}_{\text{soil-water}}} \right] \cdot \text{K}_{\text{soil-water}} \cdot \text{DEPTH}_{\text{soil}}^{-1}
\]

rate constant for leaching from soil layer:

\[
k_{\text{leach}} := \frac{\text{F}_{\text{inf soil}} \cdot \text{RAIN} \cdot \text{rate}}{\text{K}_{\text{soil-water}} \cdot \text{DEPTH}_{\text{soil}}}
\]

removal from top soil:

\[
k_{i} := k_{\text{volat}} + k_{\text{leach}} + k_{\text{bio soil}}
\]

**concentration in soil**

concentration in soil due to 10 years of continuous deposition:

\[
C_{\text{dep soil}_{10}} := \frac{D_{\text{air}}}{k_{i}} \cdot \left(1 - \exp\left(-365 \cdot \text{d} \cdot 10 \cdot k_{i}\right)\right)
\]

concentration just after the first year of sludge application:

\[
C_{\text{sludge soil}_{1}} := \frac{C_{\text{sludge}} \cdot \text{APPL}_{\text{sludge}} \cdot \text{a}}{\text{DEPTH}_{\text{soil}} \cdot \text{RHO}_{\text{soil}}}
\]

initial concentration in soil after 10 applications of sludge:

\[
C_{\text{sludge soil}_{10}} := C_{\text{sludge soil}_{1}} \cdot \left(1 + \sum_{n=1}^{9} \left(\exp\left(-365 \cdot \text{d} \cdot k_{i}^{n}\right)\right)\right)
\]
sum of the concentrations due to both processes:

\[ C_{\text{soil} \_10\_i} := C_{\text{dep} \_\text{soil} \_10\_i} + C_{\text{sludge} \_\text{soil} \_10\_i} \]

average concentration in soil over T days:

\[ \text{Clocal}_\text{soil} := \frac{D_{\text{air}}}{k_i} + \frac{1}{k_i \cdot T_i} \left( C_{\text{soil} \_10\_i} - \frac{D_{\text{air}}}{k_i} \right) \left( 1 - \exp\left( -k_i \cdot T_i \right) \right) \]

\[ \text{PEClocal}_\text{soil} := \text{Clocal}_\text{soil} + \text{PECregional}_\text{natural}_\text{soil} \]

<table>
<thead>
<tr>
<th>Clocal_soil</th>
<th>PEClocal_soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>ppm</td>
</tr>
<tr>
<td>1.285 \times 10^{-2}</td>
<td>1.337 \times 10^{-2}</td>
</tr>
<tr>
<td>1.285 \times 10^{-2}</td>
<td>1.337 \times 10^{-2}</td>
</tr>
<tr>
<td>2.029 \times 10^{-2}</td>
<td>2.081 \times 10^{-2}</td>
</tr>
</tbody>
</table>

**Indicating persistency of the substance in soil**

initial concentration after 10 years:

\[ C_{\text{soil} \_10\_i} \text{ ppm} = \begin{cases} 1.285 \times 10^{-2} \\ 1.285 \times 10^{-2} \\ 2.029 \times 10^{-2} \end{cases} \]

initial concentration in steady-state situation:

\[ \text{Face}_i := e^{-365 \cdot k_i} \]

\[ C_{\text{soil} \_\text{ss} \_i} := \frac{D_{\text{air}}}{k_i} + C_{\text{sludge} \_\text{soil} \_1\_i} \frac{1}{1 - \text{Face}_i} \]

\[ C_{\text{soil} \_\text{ss} \_i} \text{ ppm} = \begin{cases} 1.285 \times 10^{-2} \\ 1.285 \times 10^{-2} \\ 2.029 \times 10^{-2} \end{cases} \]

fraction of steady-state in soil achieved:

\[ F_{\text{st} \_\text{st} \_i} := \frac{C_{\text{soil} \_10\_i}}{C_{\text{soil} \_\text{ss} \_i}} \]

\[ F_{\text{st} \_\text{st} \_i} = \begin{cases} 1 \\ 1 \\ 1 \end{cases} \]
concentration in pore water

\[
C_{\text{local soil porew}} = \frac{C_{\text{local soil}} \cdot \rho_{\text{soil}}}{K_{\text{soil water}}}
\]

\[
P_{\text{EClolocal soil porew}} = \frac{P_{\text{EClolocal soil}} \cdot \rho_{\text{soil}}}{K_{\text{soil water}}}
\]

concentration in ground water

\[
P_{\text{EClolocal grw}} = P_{\text{EClolocal agr soil porew}}
\]
Exposure of Soil

**chemical**: Propanol  CAS-Nr.:71-23-8

**Processing of paints in paint shops**

- annual average total deposition flux:
- soil-water partitioning coefficient:
- concentration in dry sewage sludge:
- air-water partitioning coefficient:
- rate constant for for removal from top soil:
- PECregional:

**Defaults:**

- mixing depth of soil:
- bulk density of soil:
- average time for exposure:
- partial mass transfer coefficient at air-side of the air-soil interface:
- partial mass transfer coefficient at soilair-side of the air-soil interface:
- partial mass transfer coefficient at soilwater-side of the air-soil interface:
- fraction of rain water that infiltrates into soil:
- rate of wet precipitation:

```
d := 86400s
ppm := mg·kg⁻¹
a := 365·d
i := 1..3
DEPtotal_ann := 0.089·mg·m⁻²·d⁻¹
K_{soil_water} := 0.329
C_{sludge} := 0·mg·kg⁻¹
K_{air_water} := 0.000048
k_{bio_soil} := 0.023·d⁻¹
PECregional_{natural_soil} := 5.25×10⁻⁴·mg·kg⁻¹

DEPTH_soil_1 :=

0.2·m
0.2·m
0.1·m

RHO_{soil} := 1700·kg·m⁻³
T_i :=

30·d
180·d
180·d

K_{asl_air} := 120·m·d⁻¹
K_{asl_soilair} := 0.48·m·d⁻¹
K_{asl_soilwater} := 4.8×10⁻⁵·m·d⁻¹
F_{infl_{soil}} := 0.25
RAINrate := 1.92×10⁻³·m·d⁻¹
```
dry sludge application rate: \[ \text{APPL}_{\text{sludge}} := \begin{cases} 0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\ 0.5 \text{ kg m}^{-2} \text{ a}^{-1} \\ 0.1 \text{ kg m}^{-2} \text{ a}^{-1} \end{cases} \]

**Calculation:**

**aerial deposition flux per kg of soil:**
\[ D_{\text{air}} := \frac{\text{DEP}_{\text{total ann}}}{\text{DEPTH}_{\text{soil}} \cdot \text{RHO}_{\text{soil}}} \]

**rate constant for volatilisation from soil:**
\[ k_{\text{volat}} := \frac{1}{(\text{k}_{\text{soilair}} \cdot K_{\text{air_water}}) + (\text{k}_{\text{soilwater}})} \cdot K_{\text{soil_water}} \cdot \text{DEPTH}_{\text{soil}} \]

**rate constant for leaching from soil layer:**
\[ k_{\text{leach}} := \frac{\text{F}_{\text{soil}} \cdot \text{RAINrate}}{\text{K}_{\text{soil_water}} \cdot \text{DEPTH}_{\text{soil}}} \]

**removal from top soil:**
\[ k_{i} := k_{\text{volat}} + k_{\text{leach}} + k_{\text{bio soil}} \]

**concentration in soil**

**concentration in soil due to 10 years of continuous deposition:**
\[ C_{\text{dep soil}}_{10} := \frac{D_{\text{air}}}{k_{i}} \cdot (1 - \exp(-365 \cdot 10 \cdot k_{i})) \]

**concentration just after the first year of sludge application:**
\[ C_{\text{sludge soil}}_{1} := \frac{C_{\text{sludge}} \cdot \text{APPL}_{\text{sludge}}}{\text{DEPTH}_{\text{soil}} \cdot \text{RHO}_{\text{soil}}} \]

**initial concentration in soil after 10 applications of sludge:**
\[ C_{\text{sludge soil}}_{10} := C_{\text{sludge soil}}_{1} \left[ 1 + \sum_{n=1}^{9} \left( \exp(-365 \cdot k_{i}) \right)^{n} \right] \]
sum of the concentrations due to both processes:

\[ C_{\text{soil\_i\_10}} = C_{\text{dep\_soil\_i\_10}} + C_{\text{sludge\_soil\_i\_10}} \]

average concentration in soil over T days:

\[ C_{\text{local\_soil\_i}} = \frac{D_{\text{air\_i}}}{k_i} + \frac{1}{k_i \cdot T_i} \left( C_{\text{soil\_i\_10}} - \frac{D_{\text{air\_i}}}{k_i} \cdot (1 - \exp(-k_i \cdot T_i)) \right) \]

\[ \text{PEC}_{\text{local\_soil\_i}} = C_{\text{local\_soil\_i}} + \text{PEC}_{\text{regional\_natural\_soil}} \]

Indicating persistency of the substance in soil

initial concentration after 10 years:

\[
\begin{array}{c|c|c}
\text{local soil} & \text{PEC local soil} \\
\hline
8.347 \times 10^{-3} & 8.872 \times 10^{-3} \\
8.347 \times 10^{-3} & 8.872 \times 10^{-3} \\
1.318 \times 10^{-2} & 1.37 \times 10^{-2} \\
\end{array}
\]

initial concentration in steady-state situation:

\[ C_{\text{soil\_ss\_i}} = \frac{D_{\text{air\_i}}}{k_i} + C_{\text{sludge\_soil\_i\_1}} \frac{1}{1 - \text{Face}_i} \]

\[
\begin{array}{c|c|c}
\text{local soil} & \text{PEC local soil} \\
\hline
8.347 \times 10^{-3} & 8.872 \times 10^{-3} \\
8.347 \times 10^{-3} & 8.872 \times 10^{-3} \\
1.318 \times 10^{-2} & 1.37 \times 10^{-2} \\
\end{array}
\]

fraction of steady-state in soil achieved:

\[ \text{Fst\_st\_i} = \frac{C_{\text{soil\_i\_10}}}{C_{\text{soil\_ss\_i}}} \]

\[
\begin{array}{c|c|c}
\text{Fst\_st\_i} \\
\hline
1 & 1 \\
1 & 1 \\
\end{array}
\]
**concentration in pore water**

\[ C_{local\ soil\_porew} = \frac{C_{local\ soil} \cdot \text{RHO}_{soil}}{K_{soil\_water}} \]

\[ C_{local\ soil\_porew} = 4.3129 \times 10^{-2} \]

\[ C_{local\ agr\_soil\_porew} = 4.3129 \times 10^{-2} \]

\[ C_{local\ grassland\_porew} = 6.81041 \times 10^{-2} \]

\[ PEC_{local\ soil\_porew} = \frac{PEC_{local\ soil} \cdot \text{RHO}_{soil}}{K_{soil\_water}} \]

\[ PEC_{local\ soil\_porew} = 0.04584 \]

\[ PEC_{local\ agr\_soil\_porew} = 0.04584 \]

\[ PEC_{local\ grassland\_porew} = 0.07081 \]

**concentration in ground water**

\[ PEC_{local\ grw} = PEC_{local\ agr\_soil\_porew} \]
### Appendix E  Input and Output of propan-1-ol

**SimpleBox2.0a - Berechnung regionaler + kontinentaler PEC's**
- Anpassung an TGD (1996) / EUSES 1.00: Michael Feibicke (06/98)

#### Physicochemical properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Input</th>
<th>Parameter names acc. SimpleBox20</th>
<th>Unit</th>
<th>Propanol</th>
<th>Substance</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMPOUND NAME</td>
<td>[-]</td>
<td>Propanol</td>
<td>Substance</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOL WEIGHT</td>
<td>[g.mol⁻¹]</td>
<td>60.1</td>
<td>Molecular weight</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MELTING POINT</td>
<td>[°C]</td>
<td>-126.5</td>
<td>Melting Point</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VAPOR PRESSURE(25)</td>
<td>[Pa]</td>
<td>1940</td>
<td>Vapour pressure at 25°C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>log Kow</td>
<td>[log10]</td>
<td>0.34</td>
<td>Octanol-water partition coefficient</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOLUBILITY(25)</td>
<td>[mg.l⁻¹]</td>
<td>100000</td>
<td>Water solubility</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Distribution - Partition coefficients

- **Solids water partitioning (derived from K_{soil})**
  - Kp(soil)  [l.kg⁻¹]  0.086  Solids-water partitioning in soil
  - Kp(sed) [l.kg⁻¹]  0.215  Solids-water partitioning in sediment
  - Kp(susp) [l.kg⁻¹]  0.429  Solids-water partitioning in suspended matter

- **Biota-water**
  - BCF(fish) [l.kg⁻¹]  1  Bioconcentration factor for aquatic biota

#### Degradation and Transformation rates

- **Characterisation and STP**
  - PASStreadytest [y / n]  y  Characterization of biodegradability
  - Environmental **Total Degradation**
    - kdeg(air)  [d⁻¹]  2.15E-01  Rate constant for degradation in air
    - kdeg(water)  [d⁻¹]  4.70E-02  Rate constant for degradation in bulk surface water
    - kdeg(soil)  [d⁻¹]  2.30E-02  Rate constant for degradation in bulk soil
    - kdeg(sed)  [d⁻¹]  2.30E-03  Rate constant for degradation in bulk sediment

#### Sewage treatment (e.g. calculated by SimpleTreat)

- **Continental**
  - FR(volatstp) [C]  [-]  1.00E-03  Fraction of emission directed to air (STPcont)
  - FR(effstp) [C]  [-]  1.26E-01  Fraction of emission directed to wastewater (STPcont)
  - FR(sludgestp) [C]  [-]  0.00E+00  Fraction of emission directed to sludge (STPcont)

- **Regional**
  - FR(volatstp) [R]  [-]  1.00E-03  Fraction of emission directed to air (STPreg)
  - FR(effstp) [R]  [-]  1.26E-01  Fraction of emission directed to wastewater (STPreg)
  - FR(sludgestp) [R]  [-]  0.00E+00  Fraction of emission directed to sludge (STPreg)

#### Release estimation

- **Continental**
  - Edirect(air) [C]  [t.y⁻¹]  4174  Total continental emission to air
  - STPload [C]  [t.y⁻¹]  3016  Total continental emission to wastewater
  - Edirect(water1) [C]  [t.y⁻¹]  1249  Total continental emission to surface water
  - Edirect(soil3) [C]  [t.y⁻¹]  0  Total continental emission to industrial soil
  - Edirect(soil2) [C]  [t.y⁻¹]  0  Total continental emission to agricultural soil

- **Regional**
  - Edirect(air) [R]  [t.y⁻¹]  2107  Total regional emission to air
  - STPload [R]  [t.y⁻¹]  1509  Total regional emission to wastewater
  - Edirect(water1) [R]  [t.y⁻¹]  615  Total regional emission to surface water
  - Edirect(soil3) [R]  [t.y⁻¹]  0  Total regional emission to industrial soil
  - Edirect(soil2) [R]  [t.y⁻¹]  0  Total regional emission to agricultural soil
### Parameter names according SimpleBox20

<table>
<thead>
<tr>
<th>Parameter names acc. SimpleBox20</th>
<th>Uni</th>
<th>Output</th>
<th>Parameter names according Euses</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Physicochemical properties

#### Output

**- Continental**

<table>
<thead>
<tr>
<th>COMPOUND NAME</th>
<th>[-]</th>
<th>Propanol</th>
<th>Substance</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PECsurfacewater (total)</td>
<td>mg.l⁻¹</td>
<td>2.94E-04</td>
<td>Continental PEC in surface water (total)</td>
</tr>
<tr>
<td>PECsurfacewater (dissolved)</td>
<td>mg.l⁻¹</td>
<td>2.94E-04</td>
<td>Continental PEC in surface water (dissolved)</td>
</tr>
<tr>
<td>PECair</td>
<td>mg.m⁻³</td>
<td>1.13E-05</td>
<td>Continental PEC in air (total)</td>
</tr>
<tr>
<td>PECagr.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>3.49E-05</td>
<td>Continental PEC in agricultural soil (total)</td>
</tr>
<tr>
<td>PECporewater agr.soil</td>
<td>mg.l⁻¹</td>
<td>1.80E-04</td>
<td>Continental PEC in pore water of agricultural soils</td>
</tr>
<tr>
<td>PECnat.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>6.30E-05</td>
<td>Continental PEC in natural soil (total)</td>
</tr>
<tr>
<td>PECind.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>6.30E-05</td>
<td>Continental PEC in industrial soil (total)</td>
</tr>
<tr>
<td>PECsediment</td>
<td>mg.kgwwt⁻¹</td>
<td>1.93E-04</td>
<td>Continental PEC in sediment (total)</td>
</tr>
</tbody>
</table>

**- Regional**

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PECsurfacewater (total)</td>
<td>mg.l⁻¹</td>
<td>8.59E-03</td>
<td>Regional PEC in surface water (total)</td>
</tr>
<tr>
<td>PECsurfacewater (dissolved)</td>
<td>mg.l⁻¹</td>
<td>8.59E-03</td>
<td>Regional PEC in surface water (dissolved)</td>
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<td>PECair</td>
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<td>9.45E-05</td>
<td>Regional PEC in air (total)</td>
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<tr>
<td>PECagr.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>2.91E-04</td>
<td>Regional PEC in agricultural soil (total)</td>
</tr>
<tr>
<td>PECporewater agr.soil</td>
<td>mg.l⁻¹</td>
<td>1.50E-03</td>
<td>Regional PEC in pore water of agricultural soils</td>
</tr>
<tr>
<td>PECnat.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>5.25E-04</td>
<td>Regional PEC in natural soil (total)</td>
</tr>
<tr>
<td>PECind.soil</td>
<td>mg.kgwwt⁻¹</td>
<td>5.25E-04</td>
<td>Regional PEC in industrial soil (total)</td>
</tr>
<tr>
<td>PECsediment</td>
<td>mg.kgwwt⁻¹</td>
<td>5.73E-03</td>
<td>Regional PEC in sediment (total)</td>
</tr>
</tbody>
</table>
The report provides the comprehensive risk assessment of Environment part of the substance propan-1-ol. 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.

The evaluation considers the emissions and the resulting exposure to the environment and the human populations 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. For human health the scenarios for occupational exposure, consumer exposure and humans exposed via the environment have been examined and the possible risks have been identified.

The environmental risk assessment for propan-1-ol concludes that there is at present no concern for atmosphere, aquatic ecosystem, terrestrial ecosystem and for micro-organisms in the sewage treatment plant. The human health risk assessment for propan-1-ol concludes that there is at present concern for workers and consumers. There is at present no concern for humans exposed via the environment.

The conclusions of this report will lead to risk reduction measures to be proposed by the Commissions committee on risk reduction strategies set up in support of Council Regulation (EEC) No. 793/93.
The mission of the JRC is to provide customer-driven scientific and technical support for the conception, development, implementation and monitoring of EU policies. As a service of the European Commission, the JRC functions as a reference centre of science and technology for the Union. Close to the policy-making process, it serves the common interest of the Member States, while being independent of special interests, private or national.

European Commission – Joint Research Centre
Institute for Health and Consumer Protection (IHCP)
Toxicology and Chemical Substances (TCS)
European Chemicals Bureau (ECB)

European Union Risk Assessment Report

**propan-1-ol**

**Part I - environment**

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