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This investigation has been performed by order and for the account of Directorate-General for Environmental Protection, Sustainable Production Directorate (DP), within the framework of the project ‘Standard setting for other relevant substances within the WFD’.

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Abstract

Environmental Risk Limits for benzyl chloride and benzylidene chloride

RIVM has derived environmental risk limits (ERLs) for benzyl chloride and benzylidene chloride. These compounds, which might have carcinogenic potential, are used for several purposes, among which the production of dyes. They are indicated as relevant substances in the scope of the Water Framework Directive.

Environmental quality standards are used in the national policy on substances. These standards are formally set by the Dutch Steering Committee for Substances, on the basis of scientifically derived environmental risk limits (ERLs). Three routes have been taken into consideration for deriving ERLs for benzyl chloride and benzylidene chloride: direct effects on water and soil organisms, secondary poisoning of predatory birds and mammals and indirect effects on humans due to consumption of food. This latter route is critical and determines the ERLs for benzyl chloride.

For benzylidene chloride, there were not enough data to derive ERLs. However, since the current water quality standard is probably underprotective for humans, revision is needed. A risk limit for water was therefore derived on the basis of data for benzyl chloride. Benzylidene chloride might still be more toxic, the resulting value should therefore be considered as an upper limit until more information becomes available.

It is not known if the newly derived risk limits will be exceeded in surface water. The newly derived Maximum Permissible Concentrations for benzyl chloride in water (MPC_{water}) is 0.02 µg/L, which is lower than the detection limit of 0.5 µg/L. It is thus not possible to detect benzyl chloride at the level of MPC_{water}. The new MPC_{water} for benzylidene chloride of 0.0034 µg/L is even lower. Monitoring data are not available for this compound, but it is expected that concentrations are also below the detection limit.

Key words:
environmental risk limits, benzyl chloride, benzylidene chloride

Rapport in het kort

Milieurisicogrenzen voor benzylchloride en benzylideenchloride

Het RIVM heeft milieurisicogrenzen afgeleid voor benzylchloride en benzylideenchloride. Deze stoffen worden gebruikt voor industriële processen, onder ander bij de productie van kleurstoffen. De onderzochte stoffen staan op de lijst van stoffen waarvoor Nederland vanwege de Kaderrichtlijn Water nieuwe normen moet afleiden. Dat komt onder andere omdat ze mogelijk kankerverwekkend zijn.

De overheid gebruikt milieukwaliteitsnormen om het nationaal stoffenbeleid te kunnen uitvoeren. Deze normen worden vastgesteld door de Stuurgroep Stoffen, op basis van wetenschappelijk afgeleide milieurisicogrenzen. Voor de milieurisicogrenzen voor benzylchloride en benzylideenchloride zijn drie routes onderzocht: de directe effecten van deze stoffen op water- en bodemorganismen, de indirecte effecten op vogels en zoogdieren via het eten van prooidieren en de indirecte effecten op mensen via het eten van voedsel. Deze laatste route levert de laagste waarde voor benzylchloride en bepaalt daarmee de risicogrens voor deze stof.

Voor benzylideenchloride waren niet genoeg betrouwbare gegevens beschikbaar om deze routes door te rekenen. Omdat de huidige waterkwaliteitsnorm voor deze stof mogelijk niet beschermend is voor mensen, is het gewenst deze aan te passen. Daarvoor zijn gegevens over benzylchloride gebruikt, omdat dat een gelijksoortige stof is. Omdat benzylideenchloride mogelijk giftiger is dan benzylchloride, kan deze waarde nog lager worden als er nieuwe informatie beschikbaar komt.

Het is niet bekend of de nieuw afgeleid risicogrenzen in Nederlands oppervlaktewater worden overschreden. Het nieuwe MTR voor benzylchloride voor water is met 0,02 microgram per liter lager dan de concentratie die in water kan worden gemeten (0,5 microgram per liter, oftewel de detectielimiet), en kan dus niet met metingen worden aangetoond. Voor benzylideenchloride is het nieuwe MTR voor water met 0,0034 microgram per liter nog lager. Er zijn zijn geen meetgegevens beschikbaar om deze waarde te toetsen. Waarschijnlijk zijn ook hier de concentraties te laag om ze te kunnen aantonen.

Trefwoorden:
milieurisicogrenzen, benzylideenchloride, benzylchloride

Preface

The goal of this report is to derive risk limits that protect both man and the environment. This is done according to the methodology for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS), following the Guidance for the derivation of environmental risk limits within the INS framework (Van Vlaardingen and Verbruggen, 2007). This guidance incorporates the methodology of the Water Framework Directive (WFD) and TGD (EC, 2003).

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Contents

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Samenvatting

In dit rapport zijn milieurisicogrenzen afgeleid voor benzylchloride en benzylideenchloride. Beide stoffen zijn aangemerkt als relevante stoffen voor het uitvoeren van de Kaderrichtlijn Water. Benzylchloride wordt gebruikt bij de productie van benzyl-verbindingen, parfum, farmaceutische producten, kleurstoffen en kunsthars. Benzylideenchloride wordt toegepast bij de productie van verschillende chemische producten en kleurstoffen. Beide stoffen zijn mogelijk kankerverwekkend.

De overheid gebruikt milieukwaliteitsnormen voor het nationaal stoffenbeleid. Deze normen worden vastgesteld door de Stuurgroep Stoffen, op basis van wetenschappelijk afgeleide milieurisicogrenzen. Nederland onderscheidt vier milieurisicogrenzen: een niveau waarbij het risico verwaarloosbaar wordt geacht (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (MTR), het maximaal aanvaardbare niveau voor aquatische ecosystemen, specifiek voor kortdurende blootstelling ($MAC_{eco\ water}$) en een niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}).

Voor de milieurisicogrenzen voor benzylchloride en benzylideenchloride zijn drie routes onderzocht: de directe effecten van deze stoffen op water- en bodemorganismen, de indirecte effecten op vogels en zoogdieren via het eten van prooidieren en de indirecte effecten op mensen via het eten van voedsel. Er zijn geen risicogrenzen voor sediment afgeleid, omdat de stofeigenschappen hier geen aanleiding toe geven. Risicogrenzen voor lucht konden niet worden afgeleid vanwege gebrek aan gegevens.
Er waren niet voldoende betrouwbare toxiciteitsgegevens om de route van directe blootstelling van water-en bodemorganismen door te rekenen. Voor benzylchloride zijn de milieurisicogrenzen voor bodem en water op basis van indirecte blootstelling van vogels, zoogdieren en mensen wel afgeleid. De laatste route is het meest kritisch en bepaalt de uiteindelijke risicogrens.
Voor benzylideenchloride is echter ook de humaan-toxicologische informatie te beperkt om deze route door te rekenen. De huidige waterkwaliteitsnorm is mogelijk niet beschermend voor mensen en aanpassing is gewenst. Daarom is voor water een risicogrens afgeleid op basis van de gegevens voor benzylchloride. Omdat benzylideenchloride mogelijk toxischer is dan benzylchloride, moet deze waarde voorlopig als een bovengrens worden beschouwd. Een herziening kan worden overwogen wanneer nieuwe gegevens beschikbaar komen, bijvoorbeeld onder REACH.
De nu afgeleide waarden staan in Tabel 1.

In 2005 waren de concentraties van benzylchloride in de Rijn bij Lobith lager dan de detectielimiet van 0,5 µg/L. Omdat het nieuwe MTR voor water van 0,02 µg/L lager is dan deze waarde, kan er geen uitspraak worden gedaan over het al dan niet overschrijden van de risicogrenzen voor water. Voor benzylideenchloride is het nieuw afgeleide MTR voor water met 0,0034 µg/L nog lager. Er zijn geen meetgegevens beschikbaar om deze waarde te toetsen. Waarschijnlijk zijn ook hier de concentraties te laag om ze te kunnen aantonen.

Tabel 1. Milieurisicogrenzen voor benzylchloride en benzylideenchloride.

Milieurisicogrens	Eenheid	Benzylchloride	Benzylideenchloride
MTR_{water}	µg/L	2.0×10^{-2}	3.4×10^{-3}
VR_{water}	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, water}$	µg/L	n.a.	n.a.
$ER_{eco, water}$	µg/L	n.a.	n.a.
MTR_{marien}	µg/L	2.0×10^{-2}	3.4×10^{-3}
VR_{marien}	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, marien}$	µg/L	n.a.	n.a.
MTR_{bodem}	$\mu g/kg_{dwt}$	7.7×10^{-1}	n.a.
VR_{bodem}	$\mu g/kg_{dwt}$	7.7×10^{-3}	n.a.
$ER_{eco, bodem}$		n.a.	n.a.
$MTR_{dw, water}$	µg/L	2.1×10^{-2}	n.a.
MTR_{gw}	µg/L	2.1×10^{-2}	n.a.
VR_{gw}	µg/L	2.1×10^{-4}	n.a.
MTR_{lucht}	$\mu g/m^3$	n.a.	n.a.
VR_{lucht}	$\mu g/m^3$	n.a.	n.a.

n.a. = niet afgeleid vanwege gebrek aan gegevens

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Summary

In this report, environmental risk limits (ERLs) are derived for benzyl chloride and benzylidene chloride. Both compounds are appointed as relevant substances within the scope of the Water Framework Directive. Benzyl chloride is a chemical intermediate in the manufacture of benzyl compounds, perfumes, pharmaceutical products, dyes, synthetic tannins, and artificial resins. The main use of benzylidene chloride is for the production of several chemical products and dyes.

Environmental quality standards are used in the national policy on substances. These standards are formally set by the Dutch Steering Committee for Substances, on the basis of scientifically derived environmental risk limits (ERLs). Four different ERLs are distinguished in The Netherlands: a concentration at which effects are considered negligible (NC); a concentration at which no harmful effects are to be expected (maximum permissible concentration, MPC); a maximum acceptable concentration for aquatic ecosystems specifically for short-term exposure ($MAC_{eco, water}$); a concentration at which possible serious effects on the ecosystem are to be expected (serious risk concentration, SRC_{eco}).

Three routes have been taken into consideration for deriving ERLs for benzyl chloride and benzylidene chloride: direct effects on water and soil organisms; secondary poisoning of predatory birds and mammals indirect effects on humans due to consumption of food.

ERLs for sediment are not derived because the triggers to derive such limits are not met. Too little information was available to derive risk limits for air. There were not enough reliable data to include the route of direct ecotoxicity in the ERL-derivation for water and soil. For benzyl chloride, ERLs for water and soil could be derived on the basis of secondary poisoning and human consumption of fish, meat and crops. This latter route is critical and determines the ERLs for benzyl chloride.

For benzylidene chloride the human-toxicological information was too limited to derive ERLs. However, since the current water quality standard is probably underprotective for humans, revision is needed. Therefore, a risk limit for water was derived on the basis of data for benzyl chloride. This value can be revised when new data become available, *e.g.*, as a result of REACH. Resulting environmental risk limits are summarised in Table 2 below.

It is not known if the newly derived risk limits will be exceeded in surface water. Monitoring data show that in 2005, concentrations of benzyl chloride were below the detection limit of 0.5 µg/L. It is thus not possible to detect benzyl chloride at the level of the newly derived MPC_{water} of 0.02 µg/L. The new MPC_{water} for benzylidene chloride of 0.0034 µg/L is even lower. Monitoring data are not available for this compound, but it is expected that concentrations are also below the detection limit.

Table 2. Environmental risk limits as derived for benzyl chloride and benzylidene chloride.

Environmental risk limit	Unit	Benzyl chloride	Benzylidene chloride
MPC_{water}	µg/L	2.0×10^{-2}	3.4×10^{-3}
NC_{water}	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, water}$	µg/L	n.d.	n.d.
$SRC_{eco, water}$	µg/L	n.d.	n.d.
$MPC_{saltwater}$	µg/L	2.0×10^{-2}	3.4×10^{-3}
$NC_{saltwater}$	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, saltwater}$	µg/L	n.d.	n.d.
MPC_{soil}	$\mu g/kg_{dwt}$	7.7×10^{-1}	n.d.
NC_{soil}	$\mu g/kg_{dwt}$	7.7×10^{-3}	n.d.
$SRC_{eco, soil}$		n.d.	n.d.
$MPC_{dw, provisional}$	µg/L	2.1×10^{-2}	n.d.
MPC_{gw}	µg/L	2.1×10^{-2}	n.d.
NC_{gw}	µg/L	2.1×10^{-4}	n.d.
MPC_{air}	$\mu g/m^3$	n.d.	n.d.
NC_{air}	$\mu g/m^3$	n.d.	n.d.

n.d. = not derived due to lack of data

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1 Introduction

1.1 Project framework

In this report, environmental risk limits (ERLs) are derived for benzyl chloride and benzylidene chloride. The derivation of the ERLs is performed in the context of the project 'Standard setting for other relevant substances within the Water Framework Directive (WFD)', which is closely related to the project INS (International and national environmental quality standards for substances in the Netherlands). The following ERLs are considered (VROM, 2004):

- Maximum Permissible Concentration (MPC) – the concentration in an environmental compartment at which:
  - 1. no effect to be rated as negative is to be expected for ecosystems;
  - 2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);
  - 2b for humans no more than a probability of 10^{-6} per year of death can be calculated (for carcinogenic substances). Within the scope of the Water Framework Directive (WFD), a probability of 10^{-6} on a life-time basis is used.
- Negligible Concentration (NC) – the concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems must be safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC by a factor of 100.
- Maximum Acceptable Concentration (MAC_{eco}) for aquatic ecosystems – the concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Concentration for ecosystems (SRC_{eco}) – the concentration in water or soil at which possibly serious ecotoxicological effects are to be expected.

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). It should be noted that the ERLs in this report are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs). ERLs should thus be considered as preliminary values that do not have an official status.

1.2 Selection of substances and current standards

Benzyl chloride and benzylidene chloride are indicated by the Netherlands as relevant substances in the scope of the Water Framework Directive (WFD; 2000/60/EC). For these compounds, revised water quality standards have to be available by 2012 for the new river basin management plans. Both compounds are likely to be used in the Netherlands, and are pre-registered under REACH, deadline for final registration is 30 November 2010 (source European Chemicals Agency ECHA).

Current standards can be found at the website 'Risico's van stoffen' (www.rivm.nl/rvs/). For benzyl chloride an MPC of 310 µg/L is reported, based on total concentration in water. This value is most likely based on the evaluation of chlorotoluenes as performed by Van de Plassche et al. (1993). Benzylchloride, however, is not similar to chlorotoluene and in addition, the value for chlorotoluenes was based on a QSAR-approach. For air, a preliminary MPC ('ad hoc MTR') of 1.65×10^{-2} µg/m^3 is available from Hansler et al. (2008). This value is based on equilibrium partitioning using a Tolerable Daily Intake (TDI) of 5.8×10^{-3} µg/kg$_{bw}$/d as input.
The current standard for benzylidene chloride is 4.6 µg/L. This value originates from Beek (2002) and refers to a preliminary MPC ('ad hoc MTR'), based on limited data.

2 Methods

2.1 Guidance followed for ERL derivation

In this report ERLs are derived following the methodology of the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS). The methodology is described in detail in Van Vlaardingen and Verbruggen (2007), further referred to as the 'INS-Guidance'. For the aquatic compartment, this guidance implements the methodology for standard setting within the context of the WFD as developed by Lepper (2005). The methodology for derivation of the MPC for the soil compartment is based on the Technical Guidance Document (TGD) used for the European risk assessment for new and existing substances and biocides (EC, 2003). The methodology for derivation of the remaining ERLs is based on Dutch procedures. Since for the water compartment the ERL derivation according to the WFD methodology includes the derivation of an MPC protecting humans and predatory birds and mammals from adverse effects, this aspect has also been implemented in the derivation of risk limits for soil.

The process of ERL-derivation contains the following steps: data collection, data evaluation and selection, and derivation of the ERLs on the basis of the selected data. Specific items will be discussed below.

2.2 Data collection, evaluation and selection

Data of existing evaluations were used as a starting point. An on-line literature search was performed using Scopus at www.scopus.com. In addition to this, RIVM's e-tox base, EPA's ECOTOX database, IUCLID and other datasources as listed in the INS-Guidance were checked.

Information on physico-chemical properties, environmental behaviour and human toxicology, including threshold limits, was retrieved from the information sources as mentioned in the INS-Guidance. The available data on human toxicology were reviewed by a human toxicologist at RIVM.

Ecotoxicity studies were screened for relevant endpoints (i.e. those endpoints that have consequences at the population level of the test species) and thoroughly evaluated with respect to the validity (scientific reliability) of the study. A detailed description of the evaluation procedure is given in section 2.2.2 and 2.3.2 of the INS-Guidance. In short, the following reliability indices (Ri) were assigned, based on Klimisch et al. (1997):

- *Ri 1: Reliable without restriction*
  'Studies or data (…) generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline … or in which all parameters described are closely related/comparable to a guideline method.'
- *Ri 2: Reliable with restrictions*
  'Studies or data (…) (mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to

accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless well documented and scientifically acceptable.'

- *Ri 3: Not reliable*
  'Studies or data (…) in which there are interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g., unphysiologic pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for an assessment and which is not convincing for an expert judgment.'
- *Ri 4: Not assignable*
  'Studies or data (…)which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews, etc.).'

Citations
In case of (self-)citations, the original (or first cited) value was considered for further assessment, and an asterisk was added to the Ri of the endpoint that is cited.

All available studies were summarised in data-tables, that are included as Appendices to this report. These tables contain information on species characteristics, test conditions and endpoints. Explanatory notes are included with respect to the assignment of the reliability indices.

2.3 Derivation of ERLs

For a detailed description of the procedure for derivation of the ERLs, reference is made to the INS-Guidance. With respect to the terminology used and the derivation of risk limits for drinking water, additional comments should be made.

2.3.1 Terminology

In the INS-Guidance of Van Vlaardingen and Verbruggen (2007), the subscript 'marine' is used for the ERLs for the saltwater ecosystem (MPC_{marine}, $MAC_{eco,\ marine}$ etc.). In line with the forthcoming update of the WFD-methodology for derivation of water quality standards, the ERLs for the saltwater ecosystem as derived in this report are indicated with the subscript 'saltwater' ($MPC_{saltwater}$, $MAC_{eco,\ saltwater}$ etc.).

2.3.2 Drinking water

The INS-Guidance includes the MPC for surface waters intended for the abstraction of drinking water ($MPC_{dw,\ water}$) as one of the MPCs from which the lowest value should be selected as the general MPC_{water} (see sections 3.1.6 and 3.1.7 of the INS-Guidance. According to the proposal for the daughter directive Priority Substances, however, the derivation of the Annual Average Environmental Quality Standard (AA-EQS = MPC) should be based on direct exposure, secondary poisoning, and human exposure due to the consumption of fish. Drinking water was not included in the proposal and is thus not guiding for the general MPC_{water} value, the $MPC_{dw,\ water}$ is therefore presented as a separate value in this report.
The MPC_{water} is thus derived considering the individual MPCs based on direct exposure ($MPC_{eco,\ water}$), secondary poisoning ($MPC_{sp,\ water}$) or human consumption of fishery products ($MPC_{hh\ food,\ water}$); the need to derive the latter two depends on the characteristics of the compound. Although the $MPC_{dw,\ water}$ is not taken into account for the derivation of the MPC_{water}, it is used for the derivation of the groundwater risk limit, MPC_{gw}.

Related to this is the inclusion of water treatment for the derivation of the $MPC_{dw, water}$. According to the INS-Guidance (section 3.1.7), a substance specific removal efficiency related to simple water treatment should be derived in case the $MPC_{dw, water}$ is lower than the other MPCs. There is no agreement as yet on how the removal fraction should be calculated, and water treatment is therefore not taken into account.

3 Benzyl chloride

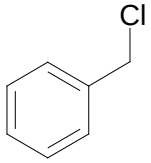
3.1 Information on production and use

Benzyl chloride is a chemical intermediate in the manufacture of benzyl compounds, perfumes, pharmaceutical products, dyes, synthetic tannins, and artificial resins (Hazardous Substances Database, HSDB, date of search 2 March 2009). The compound is marketed and/or used by several chemical companies in Europe, the use volume according to IUCLID is 100,000 – 500,000 tonnes (EC, 2000a).

3.2 Identification, physico-chemical properties, fate and distribution

3.2.1 Identity

Table 3. Identification of benzyl chloride.

Chemical name	benzyl chloride
Synonymes	alpha-chlorotoluene; (chloromethyl)benzene; chlortoluol; tolyl chloride; omega chlorotoluene; chlorophenylmethane
CAS number	100-44-7
EC number	202-853-6
Structural formula	
Molecular formula	C_7H_7Cl
SMILES code	ClCc1ccccc1

3.2.2 Physico-chemical properties

Table 4. Physico-chemical properties of benzyl chloride. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	126.59		
Water solubility	[mg/L]	460	30 °C (no details)	EC, 2000a
		525	25 °C; EPiWin; PhysProp	US EPA, 2008
		390	estimated; EpiWin; Kow	US EPA, 2008
		203	estimated; EpiWin; fragments	US EPA, 2008
pK_a	[-]		not applicable	UNEP, 1998
log K_{ow}	[-]	**2.3**	experimental	EC, 2000a
		2.3	MlogP	BioByte, 2006
		2.66	measured (shake flask), 25 °C	UNEP, 1998
		2.70	estimated; ClogP	BioByte, 2006
log K_{ow} (cont.)		2.79	estimated; EpiWin	US EPA, 2008
log K_{oc}	[-]	**2.65**	estimated; EpiWin; MCI	US EPA, 2008

Parameter	Unit	Value	Remark	Reference
		2.0	estimated; EpiWin; Kow	US EPA, 2008
Vapour pressure	[Pa]	1100	20 °C (no details)	EC, 2000a
		1300	22 °C (no details)	EC, 2000a
		164	25 °C ; EPiWin; PhysProp	US EPA, 2008
		25	0 °C (no details)	EC, 2000a
		51	10 ° (no details)	EC, 2000a
		9300	55 °C ; measured (no details)	UNEP, 1998
		19000	60 °C ; measured (no details)	UNEP, 1998
		79600	100 °C (no details)	EC, 2000a
Melting point	[°C]	-48 to -41		EC, 2000a
		-39		EC, 2000a
		-43		UNEP, 1998
		-45	EPiWin; PhysProp	US EPA, 2008
Boiling point	[°C]	177-181	at 1013 hPa	UNEP, 1998; EC, 2000a
		179		EC, 2000a
		179	EPiWin; PhysProp	US EPA, 2008
Henry's law constant	[Pa.m^3/mol]	212	estimated; EpiWin; bond	US EPA, 2008
		40.2	estimated; EpiWin; group	US EPA, 2008
		41.7	EpiWin; PhysProp	US EPA, 2008

3.2.3 Behaviour and distribution in the environment

Table 5. Selected environmental properties of benzyl chloride.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [h]	15	25 °C	EC, 2000a
		10	25 °C, pH 4	UNEP, 1998
		9.5	25 °C, pH 7	UNEP, 1998
		9.6	25 °C, pH 9	UNEP, 1998
Photolysis half-life	DT50 [h]	no information available		
Readily biodegradable	yes	71 % degradation after 14 d in activated sludge (OECD 301C)		UNEP, 1998; EC, 2000a;
Relevant metabolites	hydrolysis product is benzyl alcohol			UNEP, 1998

Table 6 summarises the partitioning over the environmental compartments as estimated by EpiWin (US EPA, 2008) using a level III fugacity model. From these estimations it appears that water, air and soil are the potentially receiving compartments.

Table 6. Estimated distribution of benzyl chloride after release to air, water and soil.

emission profile	distribution [% of total emitted]			
	air	water	soil	sediment
equal parts to air/water/soil	7.0	19	73	0.35
100 % to water	7.9	90	0.16	1.6
100 % to air	94	3.9	2.0	0.0701
100 % to soil	0.91	0.54	99	0.00962

3.2.4 Bioconcentration and biomagnification

The bioconcentration factor (BCF) and biomagnification factor (BMF) for benzyl chloride are tabulated in Table 7. No experimental bioaccumulation data were available.

Table 7. Overview of bioaccumulation data for benzyl chloride.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	18.0	Calculated using experimental log K_{OW} = 2.3	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} < 4.5.	Van Vlaardingen and Verbruggen, 2007

3.3 Human toxicology

Benzyl chloride is classified as Carc. Cat. 2; R45, T; R23, Xn; R22-48/22 and Xi; R37/38-41 in Annex 1 of Directive 67/548/EEC (ESIS, 2009). Information on human toxicology was reviewed by experts from the RIVM Centre for Substances and Integrated Risk Assessment (RIVM-SIR). The evaluation report is included in Appendix 1. Using the oral slope factor as derived by US-EPA, the additional cancer risk of 1 per 10^6 lifetime exposed people (risk-specific dose, RSD) was calculated as 6 ng/kg_{bw} d = 6 x 10^{-6} mg/kg_{bw} d. This value is similar to the TDI that was used by Hansler et al. (2008) for the derivation of an ad hoc MPC_{air}.
Using route-to-route extrapolation an inhalation risk-specific concentration (RSC) of 28 ng/m^3 can be calculated. According to the expert review, this is a provisional value because it was derived using route-to-route extrapolation, which involves considerable uncertainty. The RSC might underestimate the real inhalation risk, since benzyl chloride might act as a local alkylating agent. Therefore the potency for effects in the respiratory tract may be much higher after inhalation exposure than after ingestion. Hence, the provisional inhalation RSC of 28 ng/m^3 is only of a low to medium reliability.

3.4 Trigger values

This section reports on the trigger values for ERLwater derivation (as demanded in WFD framework).

Table 8. Benzyl chloride: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.65	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.2.2
BCF	18	[L/kg]		3.2.4
BMF	1	[kg/kg]		3.2.4
Log K_{OW}	2.3	[-]		3.2.2
R-phrases	R22,23,37/38,40,41,45,48/22	[-]		Appendix 1
A1 value	-	[µg/L]		
DW standard	-	[µg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (EC, 2003).

- benzyl chloride has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- benzyl chloride has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- benzyl chloride has a log K_{ow} < 3; assessment of secondary poisoning is not triggered.
- benzyl chloride is classified as a possible carcinogen. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) has to be derived.

- For benzyl chloride, no compound-specific A1 value or Drinking Water value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional drinking water limit is derived.

3.5 Derivation of environmental risk limits for water

3.5.1 Aquatic toxicity data

Detailed aquatic toxicity data for benzyl chloride are tabulated in Appendix 2. Endpoints for freshwater species and for marine species are reported separately. Marine species are those species that are living and tested in water with salinity > 0.5 ‰ (see section 2.2.3.11 of the INS-Guidance).
The high volatility and hydrolysis rate of benzyl chloride put special demands on the aquatic toxicity studies. In view of the fast disappearance of benzyl chloride from the test system, it was decided to accept tests without analytical verification of test concentrations only when performed in a closed system under flow-through or renewal conditions. Endpoints from static tests without analytical verification of the test substance are not considered reliable and were assigned Ri 3. An exception was made for Microtox assays with *Vibrio fischeri*, since these tests only last 5-30 minutes. The endpoints that meet these criteria are tabulated in Table 9 (freshwater species) and Table 10 (saltwater species). The results of a valid 14-days test with the guppy *Poecilia reticulata* are selected for ERL-derivation, although the preferred test duration for acute fish-studies is 96 hours.

Table 9. Benzyl chloride: selected toxicity data for freshwater species.

Chronic[a] **Taxonomic group**/*species*	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**/*species*	**L(E)C50 (mg/L)**
Crustacea		**Crustacea**	
Daphnia magna	0.1	*Daphnia magna*	3.2
		Pisces	
		Poecilia reticulata[b]	0.39

a For detailed information see Appendix 2.
b test duration 14 days.

Table 10. Benzyl chloride: selected toxicity data for marine species.

Chronic[a] **Taxonomic group**/*species*	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**/*species*	**L(E)C50 (mg/L)**
		Bacteria	
		Vibrio fischeri	1.92[b]

a For detailed information see Appendix 2.
b Test duration 5 minutes.

3.5.2 Derivation of the MPC_{water} and $MPC_{saltwater}$

3.5.2.1 Treatment of freshwater and marine data

According to Lepper (2005), data for freshwater and marine species should be pooled unless there are indications that sensitivity of species differs between the two groups. There are not enough data to make a sound comparison, and the data are combined.

3.5.2.2 $MPC_{eco, water}$ and $MPC_{eco, saltwater}$

In the absence of reliable ecotoxicity data for algae, the base set is not complete. Data on bacteria can only be used as additional data, but cannot be regarded as substitute for algae (see INS-guidance, p. 73). The SAR-estimate for algae in the program ECOSAR (included in EPIWeb; US EPA, 2008) is not considered reliable as it is based on one single experimental value from Bringmann and Kühn (1980) which is not considered reliable (see Appendix 2, Table A2.2). It is not possible to derive ERLs based on direct ecotoxicity.

3.5.2.3 $MPC_{sp, water}$ and $MPC_{sp, saltwater}$

Derivation of ERLs for secondary poisoning is not required (see section 3.4).

3.5.2.4 $MPC_{hh\ food, water}$ and $MPC_{hh\ food, saltwater}$

Derivation of the $MPC_{hh\ food, water}$ for benzyl chloride is triggered (see section 3.4). The $MPC_{hh\ food}$ is calculated using Equation 15 of the INS-Guidance. With a TL_{hh} of 6×10^{-6} mg/kg_{bw} d, the $MPC_{hh\ food}$ becomes $(0.1 \times 6 \times 10^{-6} \times 70) / 0.115 = 3.7 \times 10^{-4}$ mg/kg. Using the estimated BCF of 18 L/kg and a BMF of 1 kg/kg (section 3.2.4), the $MPC_{hh\ food, water}$ is calculated according to Equation 16 of the INS-Guidance as $3.7 \times 10^{-4} / (18 \times 1) = 2.0 \times 10^{-5}$ mg/L = 2.0×10^{-2} µg/L (based on unrounded intermediate values). This value is valid for the freshwater and for the saltwater compartment.

3.5.2.5 Selection of the MPC_{water} and $MPC_{saltwater}$

The lowest of the individual MPCs based on direct exposure, secondary poisoning or human consumption of fishery products should be selected as the final MPC. For benzyl chloride, only the $MPC_{hh\ food, water}$ is derived.

In view of the potential carcinogenicity of the compound, derivation of an ERL is considered necessary, and therefore the MPC_{water} and $MPC_{saltwater}$ are set to the $MPC_{hh\ food, water}$.

The mode of action of benzyl chloride is considered to be narcosis, and based on experience with other compounds, it can be assumed that the ERLs based on human toxicology are protective of direct ecotoxicity as well. The MPC_{water} and $MPC_{saltwater}$ are 2.0×10^{-2} µg/L.

3.5.3 $MPC_{dw, water}$

There are no official drinking water standards available. Therefore, the $MPC_{dw, water, provisional}$ is calculated according to Equation 18 of the INS-Guidance as
$(0.1 \times 6 \times 10^{-6} \times 70) / 2 = 2.1 \times 10^{-5}$ mg/L = 2.1×10^{-2} µg/L.

3.5.4 Derivation of the NC_{water} and $NC_{saltwater}$

The NC_{water} and $NC_{saltwater}$ are derived by dividing the MPC_{water} and $MPC_{saltwater}$ by a factor of 100. The NC_{water} and $NC_{saltwater}$ are 2.0×10^{-4} µg/L.

3.5.5 Derivation of the $MAC_{eco, water}$ and $MAC_{eco, saltwater}$

The base set is not complete, the $MAC_{eco, water}$ and $MAC_{eco, saltwater}$ cannot be derived.

3.5.6 Derivation of the $SRC_{eco, water}$

The base set is not complete, the $SRC_{eco, water}$ cannot be derived.

3.6 Derivation of environmental risk limits for soil

3.6.1 Derivation of the MPC_{soil}

3.6.1.1 $MPC_{eco, soil}$

There are no terrestrial toxicity data, and in the absence of an $MPC_{eco, water}$, the $MPC_{eco, soil}$ cannot be estimated by equilibrium partitioning either.

3.6.1.2 $MPC_{sp, soil}$

Derivation of the $MPC_{sp, soil}$ is not triggered, since bioaccumulation is not expected (log K_{ow} < 3 and fast hydrolysis).

3.6.1.3 $MPC_{hh\ food, soil}$

The $MPC_{hh\ food, soil}$ is derived according to the methods as described in section 3.3.6 of the INS-Guidance (Van Vlaardingen and Verbruggen, 2007). The following input values are used: TL_{hh} 6 x 10^{-6} mg/kg_{bw} d; Henry coefficient 41.7 Pa.m^3/mol, K_{oc} $10^{2.65}$ L/kg (log K_{oc} 2.65); K_{ow} $10^{2.3}$ (log K_{ow} 2.3) and water solubility 525 mg/L at 25 °C (see sections 3.2.2 and 3.3). Intermediate results of the calculation are shown in Appendix 3. The critical route is consumption of root crops. The resulting $MPC_{hh\ food, soil}$ is 0.77 µg/kg_{dwt}, based on Dutch standard soil.

3.6.1.4 Selection of the MPC_{soil}

As for water, the only route included is that based on human toxicology. The MPC_{soil} is set to 0.77 µg/kg_{dwt}, based on Dutch standard soil.

3.6.2 Derivation of the NC_{soil}

The NC_{soil} is derived by dividing the MPC_{soil} by a factor of 100. The NC_{soil} is 7.7 x 10^{-3} µg/kg_{dwt}, based on Dutch standard soil.

3.6.3 Derivation of the $SRC_{eco, soil}$

In the absence of terrestrial ecotoxicity data and an $SRC_{eco, water}$, the $SRC_{eco, soil}$ cannot be derived.

3.7 Derivation of environmental risk limits for groundwater

3.7.1 Derivation of the MPC_{gw}

3.7.1.1 $MPC_{eco, gw}$

There are no ecotoxicity data specific for groundwater species, and in the absence of an $MPC_{eco, water}$, this cannot be taken as a substitute. The $MPC_{eco, gw}$ cannot be derived.

3.7.1.2 $MPC_{human, gw}$

The $MPC_{human, gw}$ is set equal to the $MPC_{dw, water, provisional}$. The $MPC_{human, gw}$ is 2.1 x 10^{-2} µg/L.

3.7.1.3 Selection of the MPC_{gw}

The only route included is the $MPC_{human, gw}$. The MPC_{gw} is set to 2.1 x 10^{-2} µg/L.

3.7.2 Derivation of the NC_{gw}

Negligible concentrations are derived by dividing the MPC by a factor 100. The NC_{gw} is 2.1×10^{-4} µg/L.

3.7.3 Derivation of the $SRC_{eco, gw}$

The $SRC_{eco, gw}$ should be set equal to the $SRC_{eco, water}$. Since the latter could not be derived, it is not possible to set an $SRC_{eco, gw}$.

3.8 Derivation of environmental risk limits for air

3.8.1 Derivation of the MPC_{air}

3.8.1.1 $MPC_{eco, air}$

There are no ecotoxicity data for air, an $MPC_{eco, air}$, cannot be derived.

3.8.1.2 $MPC_{human, air}$

For the inhalation route no carcinogenity data are available. Using route-to-route extrapolation an inhalation risk-specific concentration (RSC) of 28 ng/m^3 can be calculated (see Appendix 1). This value involves considerable uncertainty. The RSC might underestimate the real inhalation risk, since benzyl chloride might act as a local alkylating agent. Therefore the potency for effects in the respiratory tract may be much higher after inhalation exposure than after ingestion. Hence, the reported inhalation RSC is only of low to medium reliability. Because of this, it is not considered justified to derive risk limits for air.

3.8.1.3 Selection of the MPC_{air}

In the absence of a reliable human risk limit for air, the MPC_{air} is not derived.

3.8.2 Derivation of the NC_{air}

In the absence of an MPC_{air}, the NC_{air} cannot be derived.

3.9 Comparison of derived ERLs with monitoring data

No monitoring data are available in the database of the Directorate-General for Public Works and Water Management ('Rijkswaterstaat'; www.waterbase.nl). Benzyl chloride is included in the monitoring report from the Dutch Association of River Water Companies (RIWA) over 2005, but not in the reports over 2001-2004 and 2006-2007. In 2005, concentrations in the river Rhine at Lobith were below the detection limit of 0.5 µg/L (RIWA, 2005). Since this detection limit is higher than the derived MPC_{water} of 2.0×10^{-2} µg/L, no conclusions can be drawn as to whether or not the MPC_{water} is exceeded.
Monitoring data for the other compartments are not available.

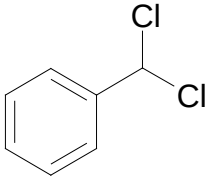
4 Benzylidene chloride

4.1 Information on production and use

Benzylidene chloride is a chemical intermediate which is used for the production of benzoyl chloride (benzene carbonyl chloride) and in the manufacture of dyes, benzaldehyde and cinnamic acid (HSDB, date of search 2 March 2009).

4.2 Identification, physico-chemical properties, fate and distribution

Table 11. Identification of benzylidene chloride.

Chemical name	benzylidene chloride
Synonymes	alpha-alpha-dichlorotoluene; (dichloromethyl)benzene; dichloromethylbenzene; dichlortoluol; benzyl dichloride; benzylene chloride; benzal chloride; dichlorophenylmethane
CAS number	98-87-3 / 29797-40-8 (see text under table)
EC number	202-709-2 / 249-854-8
Structural formula	
Molecular formula	$C_7H_6Cl_2$
SMILES code	C1=CC=C(C=C1)C(Cl)Cl

Benzylidene chloride and its synonyms are generally referred to by CAS number 98-87-3. EINECS number 202-709-2 refers to alpha-alpha-dichlorotoluene with CAS 98-87-3 (EC, 2000b), EINECS 249-854-8 to dichloromethylbenzene with CAS 29797-40-8 (EC, 2000c). The contents of the IUCLID files differ and the file for dichloromethylbenzene refers to a mixture of several dichlorotoluenes. Data from that file are therefore not used. The US EPA ECOTOX database includes both dichloromethylbenzene with CAS 29797-40-8 and (dichloromethyl)benzene with CAS 98-87-3 as a chemical entry, but does not contain ecotoxicity data.

4.2.1 Physico-chemical properties

Table 12. Physico-chemical properties of benzylidene chloride. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	161.03		
Water solubility	[mg/L]	200	20 °C; decomposition	EC, 2000b
		250	30 °C; EPiWin; PhysProp	US EPA, 2008
		390	estimated; EpiWin; Kow	US EPA, 2008
		203	estimated; EpiWin; fragments	US EPA, 2008

Parameter	Unit	Value	Remark	Reference
pK_a	[-]		not applicable	
log K_{ow}	[-]	**3.22**	estimated; ClogP	BioByte, 2006
		2.97	estimated; EpiWin	US EPA, 2008
log K_{oc}	[-]	**2.84**	estimated; EpiWin; MCI method	US EPA, 2008
		2.58	estimated; EpiWin; K_{ow} method	US EPA, 2008
Vapour pressure	[Pa]	50	20 °C	EC, 2000b
		62.7	25 °C; EPiWin; PhysProp	US EPA, 2008
		90	30 °C	EC, 2000b
		300	50 °C	EC, 2000b
Melting point	[°C]	-16		EC, 2000b
		-17	EpiWin; PhysProp	US EPA, 2008
Boiling point	[°C]	205	at 1013 hPa	EC, 2000b
		205	EpiWin; PhysProp	US EPA, 2008
Henry's law	[Pa.m^3/mol]	74.8	estimated; EpiWin; bond	US EPA, 2008
constant		**40.3**	experimental; EpiWin; PhysProp	US EPA, 2008

4.2.2 Behaviour in the environment

Table 13. Selected environmental properties of benzylidene chloride.

Parameter	Unit	Value Remark	Reference
Hydrolysis half-life	DT50 [h]	no information available	
Photolysis half-life	DT50 [h]	no information available	
Readily biodegradable	yes	89-92 % degradation after 14 d in activated sludge (OECD 301C)	EC, 2000b
		>70 % degradation after 20 d in activated sludge (OECD 301D)	EC, 2000b
		100 % degradation after 3 d in activated sludge (OECD 301E)	EC, 2000b
Relevant metabolites		no information available	

Table 14summarises the partitioning over the environmental compartments as estimated by EpiWin (US EPA, 2008) using a level III fugacity model. From these estimations it appears that water, air and soil are the potentially receiving compartments.

Table 14. Estimated distribution of benzylidene chloride after release to air, water and soil.

emission profile	distribution [% of total emitted] over			
	air	water	soil	sediment
equal parts to air/water/soil	4.2	13	82	0.50
100 % to water	8.3	88	0.40	3.4
100 % to air	90	5.2	4.4	0.20
100 % to soil	0.64	0.48	99	0.018

4.2.3 Bioconcentration and biomagnification

Bioaccumulation data for benzylidene chloride are tabulated in Table 15. No experimental bioaccumulation data were available.

Table 15. Overview of bioaccumulation data for benzylidene chloride.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	109	Calculated using log K_{OW} = 3.22	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} < 4.5.	

4.3 Human toxicology

Benzylidene chloride is classified as Carc. Cat. 3; R40, T; R23, Xn; R22 and Xi; R37/38-41 in Annex 1 of Directive 67/548/EEC (ESIS, 2009). In 1999, IARC concluded that combined exposures to alpha-chlorinated toluenes and benzoyl chloride are *probably carcinogenic to humans (Group 2A)* (IARC, 1999). Information on human toxicology was reviewed by experts from the the RIVM-SIR. The evaluation report is included in Appendix 4. Only very limited data are available regarding the human health effects of benzylidene chloride. These data do not allow for the derivation of a TDI or TCA. A similar conclusion was drawn earlier by the US EPA. In 1985 it was concluded that the existing data on benzylidene chloride are insufficient for deriving an Acceptable Daily Intake (ADI) or a carcinogenic potency factor (US EPA, 1985).

4.4 Trigger values

This section reports on the trigger values for ERLwater derivation (as demanded in WFD framework).

Table 16. Benzylidene chloride: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.74	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 4.2.2
BCF	109	[L/kg]		4.2.3
BMF	1	[kg/kg]		4.2.3
Log K_{OW}	3.22	[-]		4.2.1
R-phrases	R20,23,37/38,40,41	[-]		Appendix 4
A1 value	-	[µg/L]		
DW standard	-	[µg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (EC, 2003).

- benzylidene chloride has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- benzylidene chloride has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- benzylidene chloride has a log K_{ow} < 3; assessment of secondary poisoning is triggered.
- benzylidene chloride has a log K_{ow} < 3 combined with relevant R-phrases. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) needs to be derived.
- For benzylidene chloride, no compound-specific A1 value or Drinking Water value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional drinking water limit is derived.

4.5 Derivation of environmental risk limits for water

4.5.1 Aquatic toxicity data

Aquatic toxicity data for benzylidene chloride are tabulated in Appendix 5. Endpoints for freshwater and marine species are reported separately. Marine species are those species that are living and tested in water with salinity > 0.5 ‰ (see section 2.2.3.11 of the INS-Guidance).
As for benzyl chloride, endpoints from static tests without analytical verification of the test substance are not considered reliable and were assigned Ri 3. The only reliable endpoints were obtained for *Vibrio fischeri*, since these tests only last 5-30 minutes and are conducted in a small volume (Table 17).

Table 17. Benzylidene chloride: selected toxicity data for marine species.

Chronic[a] **Taxonomic group**/*species*	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**/*species*	**L(E)C50 (mg/L)**
		Bacteria	
		Vibrio fischeri	2.12[b]

a For detailed information see Appendix 5.
b test duration 5 minutes

4.5.2 Derivation of the MPC_{water} and $MPC_{saltwater}$

4.5.2.1 $MPC_{eco, water}$ and $MPC_{eco, saltwater}$

In the absence of reliable ecotoxicity data for algae, *Daphnia* and fish, the base set is not complete and it is not possible to derive ERLs based on direct ecotoxicity.

4.5.2.2 $MPC_{sp, water}$ and $MPC_{sp, saltwater}$

Benzylidene chloride has an estimated log $K_{ow} < 3$, thus assessment of secondary poisoning is triggered. However, since reliable chronic toxicity data for birds and mammals are not available, the $MPC_{sp, water}$ can not be calculated.

4.5.2.3 $MPC_{hh\ food, water}$ and $MPC_{hh\ food, saltwater}$

Derivation of the $MPC_{hh\ food, water}$ for benzylidene chloride is triggered (see Section 4.4). However, since a TDI is not available, the $MPC_{hh\ food, water}$ and $MPC_{hh\ food, saltwater}$ can not be calculated.

4.5.2.4 Derivation of the MPC_{water}: options for read across from benzyl chloride

The acute oral toxicity values for benzylidene chloride are roughly in the same order of magnitude as those for benzyl chloride and similar effects are reported from other human-toxicological studies. As a possible approach the human-toxicological threshold value for benzyl chloride (6 $ng/kg_{bw}/d$) might be used as a provisional value for benzylidene chloride (see Appendix 4). However, according to the expert review, the reliability of these provisional values is low considering the small database on benzylidene chloride.
The Scientific Advisory Group INS (WK-INS) concluded that the scientific basis to apply read across is too small. The resulting values would not meet the quality standards that are applied within INS for scientifically underpinned environmental risk limits. However, benzylidene chloride is on the list of relevant substances within the context of the WFD, and standards have to be available by 2012. Keeping the current ad hoc standard of 4.6 µg/L was not considered to be an option. This value is based on *Vibrio fischeri* only, and might be underprotective for humans. It was therefore advised by the WK-INS to calculate the $MPC_{hh\ food, water}$ on the basis the risk limit for benzyl chloride (see section 3.3). It is

still possible that benzylidene chloride is more toxic than benzyl chloride, and the result is thus considered as an upper limit. If the compound will be registered under REACH, additional information may become available from the dossier and adaptation of this value may then be considered.
Using the TL_{hh} of 6 x 10^{-6} mg/kg_{bw}.d the $MPC_{hh\ food}$ becomes (0.1 × 6 x 10^{-6} × 70) / 0.115 = 3.7 x 10^{-4} mg/kg. With a BCF of 109 L/kg and a BMF of 1 kg/kg (section 3.2.4), the $MPC_{hh\ food,\ water}$ and $MPC_{hh\ food,\ saltwater}$ is calculated as 3.7 x 10^{-4} / (109 × 1) = 3.4 x 10^{-6} mg/L = 3.4 x 10^{-3} µg/L (Equation 16 of the INS-Guidance). The Steering Committee for Substances is advised to set this value as an upper limit for the MPC_{water} and $MPC_{saltwater}$.

4.5.3 $MPC_{dw,\ water}$

As explained above for the MPC_{water}, the scientific basis to use the TL_{hh} of benzyl chloride as a substitute for benzylidene chloride is small. An environmental quality standard for benzylidene chloride in water is needed, because the compound is on the list of relevant substances for the Netherlands within the context of the WFD with an ad hoc MPC_{water} that is most likely underprotective. The need to derive risk limits for drinking water abstraction is, however, less apparent. It is therefore advised to postpone derivation of the $MPC_{dw,\ water}$ until information on the final registration under REACH is available. If the compound will be registered, the dossier may contain information that can be used for derivation of this risk limit.

4.5.4 Derivation of the NC_{water} and $NC_{saltwater}$

The NC_{water} and $NC_{saltwater}$ are derived by dividing the MPC_{water} and $MPC_{saltwater}$ by a factor of 100. The NC_{water} and $NC_{saltwater}$ are 3.4 x 10^{-5} µg/L.

4.5.5 Derivation of the $MAC_{eco,\ water}$ and $MAC_{eco,\ saltwater}$

The base set is not complete, the $MAC_{eco,\ water}$ and $MAC_{eco,\ saltwater}$ cannot be derived.

4.5.6 Derivation of the $SRC_{eco,\ water}$

Because no data are available, the $SRC_{eco,\ water}$ cannot be derived.

4.6 Derivation of environmental risk limits for soil

As explained above for the $MPC_{dw,\ water}$, there is no urgent need to derive risk limits for soil. It is therefore advised to postpone derivation of risk limits for soil until information on the final registration under REACH is available. If the compound will be registered, the dossier may contain information that can be used for derivation of risk limits for soil.

4.7 Derivation of environmental risk limits for groundwater and air

Similar to soil, it is advised to postpone derivation of risk limits for groundwater and air until information on the final registration under REACH is available. If the compound will be registered, the dossier may contain information that can be used for derivation of risk limits for groundwater and air.

4.8 Comparison of derived ERLs with monitoring data

No monitoring data are available in the database of the Directorate-General for Public Works and Water Management ('Rijkswaterstaat'; www.waterbase.nl). Benzylidene chloride is not included in the monitoring reports from the Dutch Association of River Water Companies (RIWA). No conclusions can be drawn as to whether or not the MPC_{water} is exceeded. It is expected, however, that the newly derived MPC_{water} of 0.0034 µg/L is lower than the detection limit. Monitoring data for the other compartments are also not available.

5 Conclusions

In this report, environmental risk limits (ERLs) are derived for benzyl chloride in water, drinking water, groundwater and soil. ERLs for sediment are not derived because the triggers to derive such limits are not breeched. Too little information was available to derive risk limits for air. There were not enough reliable ecotoxicity data to include the route of direct ecotoxicity in the ERL-derivation. Therefore, the ecosystem-based MAC and SRC could not be derived. Since the compound might have a carcinogenic potential, it was decided to derive MPCs for water and soil despite the absence of ecotoxicity data. Human exposure via food is considered to be the critical pathway for these compartments.

For benzylidene chloride, the available data did not allow for derivation of risk limits. However, water quality standards have to be available in the near future because the compound is relevant within the context of the Water Framework Directive. The current standard for this compound is probably underprotective, and using this value for water quality policy is not considered justified. It is advised to use the human-toxicological information on benzyl chloride for derivation of risk limits for benzylidene chloride in water. The resulting value is considered to be an upper limit, and may be revised. For the other compartments, it is advised to postpone derivation of risk limits until additional information becomes available, e.g., from the REACH dossier.

Resulting environmental risk limits are summarised in Table 18 below.

It is not known if the newly derived risk limits will be exceeded in surface water. Monitoring data show that in 2005, concentrations of benzyl chloride were below the detection limit of 0.5 µg/L. It is thus not possible to detect benzyl chloride at the level of the newly derived MPC_{water} of 0.02 µg/L. The new MPC_{water} for benzylidene chloride of 0.0034 µg/L is even lower. Monitoring data are not available for this compound, but it is expected that concentrations are also below the detection limit.

Table 18. Environmental risk limits as derived for benzyl chloride and benzylidene chloride.

Environmental risk limit	Unit	Benzyl chloride	Benzylidene chloride
MPC_{water}	µg/L	2.0×10^{-2}	3.4×10^{-3}
NC_{water}	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, water}$	µg/L	n.d.	n.d.
$SRC_{eco, water}$	µg/L	n.d.	n.d.
$MPC_{saltwater}$	µg/L	2.0×10^{-2}	3.4×10^{-3}
$NC_{saltwater}$	µg/L	2.0×10^{-4}	3.4×10^{-5}
$MAC_{eco, saltwater}$	µg/L	n.d.	n.d.
MPC_{soil}	$\mu g/kg_{dwt}$	7.7×10^{-1}	n.d
NC_{soil}	$\mu g/kg_{dwt}$	7.7×10^{-3}	n.d
$SRC_{eco, soil}$	$\mu g/kg_{dwt}$	n.d.	n.d.
$MPC_{dw, water, provisional}$	µg/L	2.1×10^{-2}	n.d.
MPC_{gw}	µg/L	2.1×10^{-2}	n.d
NC_{gw}	µg/L	2.1×10^{-4}	n.d
MPC_{air}	$\mu g/m^3$	n.d.	n.d.
NC_{air}	$\mu g/m^3$	n.d.	n.d.

n.d. = not derived due to lack of data

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List of terms and abbreviations

ERL	Environmental Risk Limit
INS	International and National Environmental Quality Standards for Substances in the Netherlands
MAC_{eco}	Maximum Acceptable Concentration for ecosystems
$MAC_{eco, water}$	Maximum Acceptable Concentration in freshwater
$MAC_{eco, saltwater}$	Maximum Acceptable Concentration for the saltwater environment
Marine species	Species that are living and tested in water with salinity > 0.5 ‰
MPC	Maximum Permissible Concentration
MPC_{water}	Maximum Permissible Concentration in freshwater
$MPC_{eco, water}$	Maximum Permissible Concentration in freshwater based on ecotoxicological data
$MPC_{sp, water}$	Maximum Permissible Concentration in freshwater based on secondary poisoning
$MPC_{hh\ food, water}$	Maximum Permissible Concentration in freshwater based on consumption of fish and shellfish by humans
$MPC_{dw, water}$	Maximum Permissible Concentration in freshwater based on abstraction of drinking water
$MPC_{saltwater}$	Maximum Permissible Concentration for the saltwater environment
$MPC_{eco, saltwater}$	Maximum Permissible Concentration for the saltwater environment based on ecotoxicological data
$MPC_{sp, saltwater}$	Maximum Permissible Concentration for the saltwater environment based on secondary poisoning
$MPC_{hh\ food, saltwater}$	Maximum Permissible Concentration for the saltwater environment based on consumption of fish and shellfish by humans
MPC_{soil}	Maximum Permissible Concentration in soil
$MPC_{eco, soil}$	Maximum Permissible Concentration in soil based on ecotoxicological data
$MPC_{sp, soil}$	Maximum Permissible Concentration in soil based on secondary poisoning
$MPC_{human, soil}$	Maximum Permissible Concentration in soil based on consumption of crops, milk or meat by humans
MPC_{gw}	Maximum Permissible Concentration in groundwater
$MPC_{eco, gw}$	Maximum Permissible Concentration in groundwater based on ecotoxicological data
$MPC_{human, gw}$	Maximum Permissible Concentration in groundwater based on human toxicological data
MPC_{air}	Maximum Permissible Concentration in air
$MPC_{eco, air}$	Maximum Permissible Concentration in air based on ecotoxicological data
$MPC_{human, air}$	Maximum Permissible Concentration in air based on human toxicological data
NC	Negligible Concentration
NC_{water}	Negligible Concentration in freshwater
$NC_{saltwater}$	Negligible Concentration for the saltwater environment
NC_{soil}	Negligible Concentration in soil
NC_{gw}	Negligible Concentration in groundwater
NC_{air}	Negligible Concentration in air
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals (1907/2006/EC)

RSD	Risk Specific Dose, human toxicological risk limit referring to a specified risk level
SRC_{eco}	Serious Risk Concentration for ecosystems
$SRC_{eco, water}$	Serious risk concentration for freshwater ecosystems
$SRC_{eco, soil}$	Serious risk concentration for terrestrial ecosystems
WFD	Water Framework Directive (2000/60/EC)

Appendix 1. Derivation of human MPCs for benzylchloride

The following is a copy of the RIVM-SIR expert advice by B. Tiesjema, dated 15 April 2009

1. Introduction

Benzyl chloride (synonyms alpha-chlorotoluene, chloromethylbenzene and chlorophenylmethane, CAS 100-44-7) is a colourless to slightly yellow liquid with a pungent odour and does not occur as such in nature. It is produced on site by photochlorination of toluene and it is used for the manufacture of benzyl compounds, perfumes, pharmaceutical products, dyes, synthetic tannins, and artificial resins. Benzyl chloride is poorly soluble in water (525 mg/L, see section 3.2.2), but rapidly hydrolyses to benzyl alcohol in water phase in a temperature dependent manner, and is readily biodegradable. For benzyl chloride, a vapour pressure of 9.3×10^3 Pa and 1.9×10^4 Pa is reported at 55 °C and at 60 °C, respectively. The major route of exposure is inhalation, but it can also be absorbed into the body through the skin and by ingestion (UNEP, 1998; EC, 2000a; HSDB, 2005; NIOSH, 1978). Benzyl chloride is classified as Carc. Cat. 2; R45, T; R23, Xn; R22-48/22 and Xi; R37/38-41 in Annex 1 of Directive 67/548/EEC (ECB website, 2009).

2. Toxicology

Toxicokinetics

Absorption

Benzyl chloride is absorbed through lung and gastrointestinal tract (not further specified) (HSDB, 2005).

Distribution

In the rat, 48 hours after an oral dose, benzyl chloride is distributed to the stomach, gastric contents, ileum and duodenum, followed by liver, adrenal, bone marrow and blood (HSDB, 2005). Female rats maintain a slightly lower tissue concentration (with the exception of blood and kidneys) than males (HSDB, 2005).

Metabolism

Benzyl chloride is metabolized to mercapturic acid, benzyl alcohol, and benzaldehyde (UNEP, 1998).

Excretion

Within 72 hours following oral administration to the rat, approximately 76 % of the initial dose is excreted in urine as benzyl chloride or benzyl chloride metabolites, while 8.3 % is expired in air as CO_2, benzyl chloride or benzyl chloride metabolites (UNEP, 1998). Female rats excrete ^{14}C-labelled benzyl chloride at a higher rate than males (HSDB, 2005).

Toxicity

Irritation and sensitization

Benzyl chloride has been shown to induce skin, eye and respiratory tract irritation in rabbits, mice and rats. Concentrations exceeding 0.1 mg/L benzyl chloride for two hours in rats and mice exhibited irritation of the eyes, nose, and throat and decreased respiratory rate (OEHHA, 1999). In addition skin sensitization has been reported (UNEP, 1998). Also in humans inhalation of benzyl chloride causes

severe irritation of the upper respiratory tract, skin, eyes, and mucous membranes, and lung damage along with pulmonary oedema (fluid in lungs) (US-EPA, 2000). Exposure to 160 mg/m³ benzyl chloride for five minutes was reported to be unbearably irritating to the eyes and respiratory tract; a five minute exposure to 6-8 mg/m³ benzyl chloride resulted in 'slight conjunctivitis' (OEHHA, 1999). Ingestion of benzyl chloride by humans may cause severe burns of the mouth, throat, and gastrointestinal tract resulting in nausea, vomiting, cramps, and diarrhoea. (US-EPA, 2000).

Acute and subacute toxicity

LC_{50} and LD_{50} values found in rat and mouse studies are summarized below.

Species	**Dose**	**Criterion**	**Exposure route**	**Reference**
Rat, male	1231 mg/kg bw	LD_{50}	oral, single dose	UNEP, 1998
Mouse	1500 mg/kg bw	LD_{50}	oral, single dose	UNEP, 1998
Rat	340-380 mg/kg bw	LD_{50}	oral, single dose	EC, 2000a
Rat, male	440 mg/kg bw	LD_{50}	oral, single dose	EC, 2000a
Mouse, male	1620 mg/kg bw	LD_{50}	oral, single dose	EC, 2000a
Mouse	780 mg/kg bw	LD_{50}	oral, single dose	EC, 2000a
Mouse	625 mg/kg bw	LD_{50}	oral, single dose	EC, 2000a
Rat , male and female	> 4.05 mg/L	LC_{50}	1 h inhalation	EC, 2000a
Rat , male	~ 3.5 mg/L	LC_{50}	4 h inhalation	EC, 2000a
Rat , female	> 4.09 mg/L	LC_{50}	4 h inhalation	EC, 2000a
Rat	0.74 mg/L	LC_{50}	4 h inhalation	EC, 2000a
Rat , male	> 0.1 mg/L	LC_{50}	2 h inhalation	EC, 2000a
Rat	> 0.5 mg/L	LC_{50}	1 h inhalation	EC, 2000a
Rat , male and female	1.79 mg/L	LC_{50}	4 h inhalation	EC, 2000a
Mouse	0.39 mg/L	LC_{50}	2 h inhalation	EC, 2000a
Mouse	> 0.5 mg/L	LC_{50}	1 h inhalation	EC, 2000a
Rat	740 mg/m^3 (150 ppm)/2 hr	LC_{50}	2 h inhalation	Mikhailova, 1965, cited in OEHHA, 1999
Rat	1970 mg/m^3 (400 ppm)/1 hr	LC_0	1 h inhalation	UNEP, 1998
Mouse	390 mg/m^3 (80 ppm)/2 hr	LC_{50}	2 h inhalation	Mikhailova, 1965, cited in OEHHA, 1999
Mouse	1970 mg/m^3	LC_0	1 h inhalation	UNEP, 1998

Subchronic and chronic toxicity

Repeated inhalation exposure in mice results in pathological changes in both the anterior respiratory epithelium adjacent to vestibule and the olfactory epithelium in the dorsal meatus, with a NOEL of 107 mg/m^3. Repeated oral exposure in rats (26 weeks) induces severe gastritis of the forestomach, often with ulcers. In addition, acute myocardial necrosis and oedema of the heart are also observed frequently. Symptoms finally cause death. A NOEL of 12.9 mg/kg/day was reported for males and 6.4 mg/kg/day for females (UNEP, 1998).

Reproduction and development

In an oral teratogenic study in female rats at doses of 0, 50, 100 mg/kg/ bw/day from day six through day fifteen of gestation, no general toxicity was reported. In addition, no effects on fertility were observed. In pups foetal length was reduced at 100 mg/kg bw/day, but no major treatment-induced skeletal or visceral abnormalities were noted. In male mice, small increases in sperm head abnormalities were observed at lethal doses (500 mg/kg after subcutaneous administration and 200 mg/kg bw/day after intraperitoneal administration (UNEP, 1998).

Genotoxicity and carcinogenicity

Benzyl chloride is weakly genotoxic. It is mutagenic to some sensitive strains of *Salmonella typhimurium* and *Escherichia coli*, but not to others. In addition, in several mammalian cell types (mouse and hamster), induction of mutations has been observed at the HGPRT and TK locus and it was weakly positive in an *in vitro* micronucleus test. In rat liver cells chromatid-type aberrations were observed, although chromosomal aberrations could not be found in human lymphocytes (HSE, 1998). Sister chromatid exchanges of CHO cells (HSE, 1998) are also reported (doses 10-25 µg/ml, no metabolic activation). In cultured human cells, benzyl chloride induced DNA strand breaks but not unscheduled DNA synthesis or chromosomal aberrations (UNEP, 1998). Several *in vivo* bone marrow micronucleus-tests in mice however were negative (oral dose levels up to 876 mg/kg bw) (HSE, 1998). Recent publications indicate that the weakness of the mutagenic response of benzyl chloride in bacteria may be due to the volatile nature of the compound and may increase when appropriate test methods for the evaluation of volatile compounds are used (Fall et al. 2006 and 2007).
In a NCI carcinogenicity bioassay, rats and mice were administered benzyl chloride in corn oil by gavage 3 times/week for 104 weeks (rats received either 0, 15, or 30 mg/kg per dose; mice received either 0, 50, or 100 mg/kg per dose). Dose-dependent increases were observed in thyroid C-cell adenoma/carcinoma in female rats (4/52, 8/51, 14/52 for low, medium and high doses, respectively), hemangioma/ hemangiosarcoma in male mice (0/52, 0/52, 5/52), forestomach carcinoma/papilloma in male mice (0/51, 4/52, 32/52), lung alveolarbronchiolar adenoma/carcinoma in female mice (1/52, 2/51, 6/51) and forestomach carcinoma/papilloma in female mice (0/52, 5/50, 19/51). In addition, hepatocellular carcinoma/ adenomas (17/52, 28/52, 20/51) were observed in a non dose-dependent manner in male mice (UNEP, 1998, US-EPA, 1994). Small cohort studies of occupational exposures to alpha-chlorinated toluenes and benzoyl chloride in the United States and England each noted an approximately three-fold excess of lung cancer (IARC, 1999).

3. Evaluation by other organisations

In their evaluation in 1994, US EPA concluded that the existing data on benzyl chloride are inadequate to determine an inhalation RfC. Based on significantly increased incidences of benign and malignant tumors at multiple sites in both sexes of mice and a significant increase in thyroid tumors in female rats, US-EPA has classified benzyl chloride as B2; probable human carcinogen. They estimated an oral slope factor of 1.7E-1 per (mg/kg)/day (US EPA, 1994).

IARC concluded in 1999 that here is *sufficient evidence* in experimental animals for the carcinogenicity of benzyl chloride. In addition, they concluded that combined exposures to alpha-chlorinated toluenes and benzoyl chloride are *probably carcinogenic to humans (Group 2A)* (IARC, 1999).

4. Evaluation

Benzyl chloride has shown carcinogenic effects after oral exposure. Genotoxicity results indicate some genotoxic potential *in vitro*. Chromosomal aberrations were found, as well as increased mutation frequencies, micronucleus induction and sister chromatid exchanges. Available *in vivo* studies were negative. Because in these *in vivo* studies, however, micronuclei in bone marrow were the only

endpoint examined, uncertainty remains concerning the genotoxicity *in vivo* and consequently concerning the mode of action for tumour formation (genotoxic or not). Based on this a non-threshold approach is considered appropriate. Using the oral slope factor as derived by US-EPA the additional cancer risk of 1 per 10^6 lifetime exposed people (risk-specific dose (RSD)) can be calculated. An oral exposure to 6 ng benzyl chloride/kg bw/day would result in an additional cancer risk of 1 per 10^6 lifetime exposed people.
For the inhalation route no carcinogenity data are available. In absence of any data for the carcinogenic potency of benzyl chloride after inhalation, a similar activity via inhalation is assumed as via oral intake. Using route-to-route extrapolation an inhalation risk-specific concentration (RSC) of 28 ng/m^3 can be calculated[1]. This is a provisional value because it was derived using route-to-route extrapolation, which involves considerable uncertainty. It should be noted that the RSC might underestimate the real inhalation risk, since benzyl chloride might act as a local alkylating agent. Therefore the potency for effects in the respiratory tract may be much higher after inhalation exposure than after ingestion. Hence, the provisional inhalation RSC is only of a low to medium reliability.

5. Conclusion

Compound	**RSD_{oral}**	**$pRSC_{inhalation}$ ***
Benzyl chloride	6 ng/kg bw/day	28 ng/m^3

* provisional value because it was derived using route-to-route extrapolation

[1] It is assumed that absorption via the inhalational route is 75 % of that of the oral route. Using the standard values for adult body weight (70 kg) and daily ventilation volume (20 m3/day), the RSC can be calculated as follows:
RSC = (RSD*70/20)*100/75

Appendix 2. Detailed aquatic toxicity data for benzyl chloride

Legend to column headings	
A	test water analysed Y(es)/N(o)
Test type	S = static; Sc = static closed; R = renewal; F = flow through; CF = continuous flow; IF = intermittent flow system
Purity	refers to purity of active substance or content of active in formulation
Test water	am = artificial medium; dtw = dechlorinated tap water; dw = deionised/dechlorinated/distilled water; nw= natural water; rw = reconstituted water; rtw = reconstituted tap water; tw = tap water
T	temperature
Ri	Reliability index according to Klimisch et al. (1997); asterisk indicates citation

Table A2.1 Acute toxicity data for freshwater species

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T	Hardness CaCO3 [mg/L]	Exp time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae																
Pseudokirchneriella subcapitata		Y	Sc	benzyl chloride	99.9					72 h	EC50	biomass	19.3	3	1,2,3,4	UNEP, 1998
Crustacea																
Daphnia magna	<24 h, 0.315-0.630 mm	N	S	benzyl chloride		tw	7.6-7.7	20-22	286	24 h	EC50	immobility	8.4	3	5	Bringmann and Kühn, 1977
Daphnia magna	<24 h, Strauss, IRCHA	N	S	benzyl chloride		am	8.0±0.2	20	250	24 h	EC50	immobility	1.3	3	5	Bringmann and Kühn, 1982
Daphnia magna		N	R	benzyl chloride	99.9					48 h	EC50	immobility	3.2	2	2,6,7	UNEP, 1998
Pisces																
Danio rerio		N	S	benzyl chloride			7.5 ± 0.3			96 h	LC50	mortality	3.9	3	8,9	Wellens, 1982
Leuciscus idus melanotus	1.5 ± 0.3 g, 5 - 7 cm	N	S	benzyl chloride		dtw	7 - 8	20 ± 1	267 ± 53	48 h	LC50	mortality	3	3	8,9	Juhnke and Lüdemann, 1978
Leuciscus idus melanotus	1.5 ± 0.3 g, 5 - 7 cm	N	S	benzyl chloride		dtw	7 - 8	20 ± 1	267 ± 53	48 h	LC50	mortality	4.5	3	8,9	Juhnke and Lüdemann, 1978
Leuciscus idus melanotus				benzyl chloride						48 h	LC50	mortality	22-24	4	8,9,10	EC, 2000a
Leuciscus idus melanotus		N	S	benzyl chloride			7.5 ± 0.3			96 h	LC50	mortality	16	3	8,9,11	Wellens, 1982
Oryzias latipes		N	R	benzyl chloride	99.9					24 h	LC50	mortality	7.5	3	12,13,14	UNEP, 1998
Oryzias latipes		N	R	benzyl chloride	99.9					48 h	LC50	mortality	4.2	3	12,13,14	UNEP, 1998
Oryzias latipes		N	R	benzyl chloride	99.9					72 h	LC50	mortality	2.4	3	12,13,14	UNEP, 1998
Oryzias latipes		N	R	benzyl chloride	99.9					96 h	LC50	mortality	1.9	3	12,13,14	UNEP, 1998
Pimephales promelas	3.2-4.2 cm	Y	S	benzyl chloride		rw	7.2-7.9	22	40-48	24 h	LC50	mortality	11.6	3	8,15	Curtis et al., 1979
Pimephales promelas	3.2-4.2 cm	Y	S	benzyl chloride		rw	7.2-7.9	22	40-48	48 h	LC50	mortality	7.3	3	8,15	Curtis et al., 1979
Pimephales promelas	3.2-4.2 cm	Y	S	benzyl chloride		rw	7.2-7.9	22	40-48	96 h	LC50	mortality	4.7-7.8	3	8,15,16	Curtis et al., 1979
Pimephales promelas	3.2-4.2 cm	Y	S	benzyl chloride		rw	7.2-7.9	22	40-48	96 h	LC50	mortality	4.7-7.8	3*	8,15,16	Curtis and Ward, 1981
Pimephales promelas			S	benzyl chloride		rw	7.2-7.6	22	40-48	24 h	LC50	mortality	12.5	3	8,17	EC, 2000a
Pimephales promelas			S	benzyl chloride		rw	7.2-7.9	22	40-48	96 h	LC50	mortality	5	3	8,17	EC, 2000a
Poecilia reticulata	2-3 m	N	R	benzyl chloride	>99	rw		22	25	14 d	LC50	mortality	0.39	2	18,19	Hermens et al., 1985
Poecilia reticulata	2-3 m	N	R	benzyl chloride		rw		22	25	14 d	LC50	mortality	0.39	2*	18,19,20	UNEP, 1998

Notes
1 according to OECD 201 (1984)
2 closed system; concentrations not measured
3 analysis performed but endpoint based on nominal, no information on actual concentrations
4 solvent Tween 80/acetone (1:1) or DMSO/HCO-40 (9:1); solvent concentration given as "minimal amount"; solvent control probably not included
5 systems closed with filterpaper
6 according to OECD 202; not GLP

7 solvent DMSO/HCO-40 (4:1; 10-100 mg/L); solvent control included
8 unknown if closed systems were used
9 according to German standard test methods (1974)
10 values as reported in IUCLID cannot be reproduced from original reference
11 according to OECD (draft), UBA 2.6 and EG C5.1.1-test methods
12 according to OECD 203
13 open system
14 solvent DMSO/HCO-40 (4:1; 10 mg/L); solvent control included
15 concentrations analysed, but endpoint based on nominal concentrations while other tests indicate that majority is lost from system
16 range based on 30% mortality at 4.5 mg/L and 100% at 7.8 mg/L
17 original reference could not be retrieved
18 glass covered, daily renewal
19 test conditions described in Könemann H. 1981. Quantitative structure activity relationships in fish toxicity studies. Part 1: Relationship for 50 industrial pollutants. Toxicology 19: 209-221
20 according to SIDS, value originates from Könemann, 1981 (see note 19), but cannot be retrieved from that reference; most likely Hermens et al., 1985 is meant.

Table A2.2 Chronic toxicity data for freshwater species

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T	Hardness CaCO3 [mg/L]	Exp time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria																
Pseudomonas putida		N	S			am	7.0	25	81	16 h	NOEC	growth inhibition	4.80	3	1,2	Bringmann and Kühn, 1980a
Cyanobacteria																
Microcystis aeruginosa		N	S	benzylchloride		am	7.0	27	55	8 d	NOEC	growth inhibition	30	3	1,2	Bringmann and Kühn, 1978a
Microcystis aeruginosa		N	S	benzylchloride		am	7.0	27	55	8 d	NOEC	growth inhibition	30	3*	2,3	Bringmann and Kühn, 1978b
Protozoa																
Entosiphon sulcatum		N	S	benzylchloride		am	6.9	25	75	72 h	NOEC	growth inhibition	25	3	2,3	Bringmann, 1978
Entosiphon sulcatum		N	S	benzylchloride		am	6.9	25	75	72 h	NOEC	growth inhibition	25	3*	1,2	Bringmann and Kühn, 1980a
Entosiphon sulcatum											NOEC	growth inhibition	25	3*	2,3,4	Bringmann and Kühn, 1981
Chilomonas paramaecium		N	S	benzylchloride		am	6.9	20	75	48 h	NOEC	growth inhibition	> 40	3	2,3	Bringmann et al., 1980
Chilomonas paramaecium											NOEC	growth inhibition	> 40	3*	2,3,4	Bringmann and Kühn, 1981
Uronema parduczi		N	S	benzylchloride		am	6.9	25	75	20 h	NOEC	growth inhibition	50	3	2,3	Bringmann and Kühn, 1980b
Uronema parduczi											NOEC	growth inhibition	50	3*	2,3,4	Bringmann and Kühn, 1981
Algae																
Scenedesmus quadricauda		N	S	benzylchloride		am	7.0	27	55	8 d	NOEC	growth inhibition	50	3	1,2	Bringmann and Kühn, 1978a
Scenedesmus quadricauda		N	S	benzylchloride		am	7.0	27	55	8 d	NOEC	growth inhibition	50	3*	2,3	Bringmann and Kühn, 1978b
Scenedesmus quadricauda		N	S	benzylchloride		am	7.0	27	55	8 d	NOEC	growth inhibition	50	3*	1,2	Bringmann and Kühn, 1980a
Pseudokirchneriella subcapitata		Y	Sc	benzylchloride						72 h	NOEC	biomass	10	3	5,6,7,8	UNEP, 1998
Crustacea																
Daphnia magna		N	R	benzylchloride	99.9	dtw	7.6-8.0		48-111	21 d	NOEC	reproduction	0.1	2	5,9,10	UNEP, 1998

Notes
1 endpoint Toxic Threshold is considered as a NOEC
2 not analysed, unknown if closed systems were used
3 endpoint Toxische GrenzKonzentration (TGK) is considered as a NOEC
4 test conditions described in first cited reference
5 closed system; concentrations not measured
6 analysed but endpoint based on nominal, no information on actual concentrations
7 solvent Tween 80/acetone (1:1) or DMSO/HCO-40 (9:1); solvent concentration given as "minimal amount"; solvent control probably not included

8 according to OECD 201 (1984)
9 according to OECD 202; not GLP
10 solvent DMSO/HCO-40 (4:1; 3.2 mg/L); solvent control included

Table A2.3 Acute toxicity data for marine species

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T	Salinity [‰]	Exp time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria																
Vibrio fischeri		N	S		97%		5-8	15		5 min	EC50	bioluminescence	1.92	2	1,2,3	Kaiser and Ribo, 1988
Vibrio fischeri		N	S		97%		5-8	15		5 min	EC50	bioluminescence	1.92	2*	1,2	Kaiser and Palabrica, 1991
Vibrio fischeri		N	S		97%		5-8	15		15 min	EC50	bioluminescence	2.25	2	1,2	Kaiser and Ribo, 1988
Vibrio fischeri		N	S		97%		5-8	15		15 min	EC50	bioluminescence	2.25	2*	1,2	Kaiser and Palabrica, 1991
Vibrio fischeri		N	S		97%		5-8	15		30 min	EC50	bioluminescence	2.97	2	1,2	Kaiser and Ribo, 1988
Vibrio fischeri		N	S		97%		5-8	15		30 min	EC50	bioluminescence	2.97	2*	1	Kaiser and Palabrica, 1991
Vibrio fischeri		N	S		97%		5-8	15		30 min	EC50	bioluminescence	2.98	2*	1,6	EC, 2000a
Crustacea																
Penaeus setiferus	juv.	Y	S			am	8.3-8.7	22	40-48	24 h	LC50	mortality	7.1	3	1,4	Curtis et al., 1979
Penaeus setiferus	juv.	Y	S			am	8.3-8.7	22	40-48	48 h	LC50	mortality	4.4	3	1,4	Curtis et al., 1979
Penaeus setiferus	juv.	Y	S			am	8.3-8.7	22	40-48	96 h	LC50	mortality	3.9	3	1,4	Curtis et al., 1979
Penaeus setiferus	juv.	Y	S			am	8.3-8.7	22	40-48	96 h	LC50	mortality	0.14	3	1,5	Curtis et al., 1979

Notes
1 not reported whether systems are closed
2 EC50 recalculated from reported log (L/mmol)
3 methods described in Ribo JM, Kaiser KLE. 1987. Photobacterium phosphoreum toxicity bioassay. I. Test procedures and applications. Toxic Assess 2: 305-323
4 concentrations analysed, endpoint based on nominal concentrations while analytical data indicate that majority is lost from system
5 based on measured concentrations, but not reported whether this refers to initial, end or mean
6 original reference could not be retrieved

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Appendix 3. Intermediate results for the $MPC_{human, soil}$ of benzyl chloride

Declaration of Variables	Value	Explanation	Unit
ALPHA	1.434E+03	sink term of differential equation	[d-1]
BAFmeat	5.012E-06	bioaccumulation factor for meat	[d.kgmeat-1]
BAFmilk	7.943E-06	bioaccumulation factor for milk	[d.kgmilk-1]
BETAagric	3.514E-05	source term of differential equation, agricultural soil	[kgc.m-3.d-1]
Cair	0.000E+00	concentration in air	[kgc.m-3]
Cagric,porew leaf_temp	8.023E-05	concentration in pore water of agricultural soil, calculated from Cleaf not compared with water solubility	[kgc.m-3]
Cagric,porew root_temp	2.894E-08	concentration in pore water of agricultural soil, calculated from Croot not compared with water solubility	[kgc.m-3]
Cagric,porew leaf	8.023E-05	concentration in pore water of agricultural soil, calculated from Cleaf, compared with water solubility	[kgc.m-3]
Cagric,porew root	2.894E-08	concentration in pore water of agricultural soil, calculated from Croot, compared with water solubility	[kgc.m-3]
Cleaf	3.500E-11	concentration in leaves of plant	[kgc.kgwwt-1]
Cmeat	1.395E-10	concentration in meat	[kgc.kgwwt-1]
Cmilk	7.487E-11	concentration in dairy products	[kgc.kgwwt-1]
Croot	1.094E-10	concentration in root tissue of plant	[kgc.kgwwt-1]
Fassaer	0.000E+00	fraction of substance adsorbed to aerosol	[-]
Icgrass	6.760E+01	daily intake of grass (wet weight)	[kgwwt.d-1]
Icsoil	4.647E-01	daily intake of soil (wet weight)	[kgwwt.d-1]
Kair-water	1.760E-02	air-water partition coefficient	[m3.m-3]
kelimplant	0.000E+00	rate constant for total elimination in plants	[d-1]
Kleaf-air	1.506E+02	partition coeff. between leaves and air	[m3.m-3]
Kplant-water	2.645E+00	partition coeff. between plant tissue and water	[m3.m-3]
Kp soil	8.934E-03	solids-water partition coefficient in soil	[m3.kg-1]
Ksoil-water	1.360E+01	total soil-water partition coefficient	[m3.m-3]
Q milk	5.473E+01	substitution factor	
Q meat	5.473E+01	substitution factor	
TSCF	8.759E-01	transpiration-stream concentration factor	[-]
MPChuman,soil leaf SI	6.420E-07	maximum permissible concentration in soil based on leaf cons. in SI units	[kg.kgwwt-1]
MPChuman,soil root SI	2.316E-10	maximum permissible concentration in soil based on root cons. in SI units	[kg.kgwwt-1]
MPChuman,soil milk SI	2.012E-05	maximum permissible concentration in soil based on milk cons. in SI units	[kg.kgwwt-1]
MPChuman,soil meat SI	5.944E-05	maximum permissible concentration in soil based on meat cons. in SI units	[kg.kgwwt-1]

Appendix 4. Derivation of human MPCs for benzylidene chloride.

The following is a copy of the RIVM-SIR expert advice by B. Tiesjema, dated 15 April 2009.

1. Introduction

Benzylidene chloride (CAS no 98-87-3 or 29797-40-8; synonyms alpha-alpha-dichlorotoluene, benzyl dichloride, benzal chloride, dichlortoluol, dichloromethylbenzene and dichlorophenylmethane) is a colourless oily liquid with a pungent odour. It is produced by reaction of dichlorocarbene (CCl_2) with benzene and its main use is for the production of benzoyl chloride. It is also used in the manufacture of dyes, benzaldehyde and cinnamic acid. Benzylidene chloride is poorly soluble in water (250 mg/L, see section 4.2.1) in water, but soluble in dilute alkali and in most organic solvents. For benzylidene chloride, a vapour pressure of 133 Pa is reported at 35.4 °C. Exposure to benzylidene chloride occurs by inhalation of its aerosol and by ingestion (ICSC, 2000; HSDB, 2003; IARC, 1999). Benzylidene chloride is classified as Carc. Cat. 3; R40, T; R23, Xn; R22 and Xi; R37/38-41 in Annex 1 of Directive 67/548/EEC (ECB website, 2009).

2. Toxicology

2.1 Toxicokinetics

No data are available with regard to the toxicokinetics of benzylidene chloride.

2.2 Toxicity

Irritation and sensitization

A single two hour exposure of mice and rats to benzylidene chloride (100 mg/m^3) produced irritation of the eyes and respiratory mucosa and slowed respiration (IARC, 1982). Irritation to skin (strong) and eye (slight) in rabbits was also reported (EC, 2000b). In addition, benzylidene chloride vapors are irritating to the eyes in humans (HSDB, 2003).

Acute and subacute toxicity

LC_{50} and LD_{50} values found in rat and mouse studies are summarized below.

Species	Dose	Criterion	Exposure route	Reference
Rat	3250 mg/kg	LD_{50}	oral, single dose	Vernot, 1977
Mouse	2460 mg/kg	LD_{50}	oral, single dose	Vernot, 1977
Rat	2250 mg/kg	LD_{50}	oral, single dose	EC, 2000b
Mouse	1400 mg/kg	LD_{50}	oral, single dose	EC, 2000b
Rat	0.4 mg/L	LC_{50}	2 h inhalation	EC, 2000b
Rat	4.3 mg/L	LC_{50}	4 h inhalation	EC, 2000b
Mouse	0.21 mg/L	LC_{50}	2 h inhalation	EC, 2000b

A single two hour exposure of mice and rats to benzylidene chloride (100 mg/m^3) produced central nervous system excitation. Hyperemia of the extremities was also noted; at 1000 mg/m^3 mice exhibited motor automatism, while rats showed twitching of peripheral muscles (IARC, 1982).

Subchronic and chronic toxicity

When rats were exposed to 0.1 mg/L of benzylidene chloride in an inhalation chamber for one month, body weight loss was similar as observed in the acute studies (IARC, 1982).

Reproduction and development

No data available.

Genotoxicity and carcinogenicity

Benzylidene chloride was mutagenic in mutation assays using *Salmonella typhimurium* strain TA100 (the only strain tested) and in *Escherichia coli strain* WP2 hcr, with metabolic activation (Arochlor 1254 microsomal liver fraction). In addition, it was positive in a recombination assay with *Bacillus subtilis* (IARC, 1982).

Benzylidene chloride (in benzene) was tested by skin application (~ 75-100 mg/kg body weight) in female mice, twice weekly for 50 weeks. From the 19 treated mice 14 had died by the end of the experiment; 12 developed tumors: nine with squamous cell carcinomas of the skin ($p < 0.01$), two with skin fibrosarcoma, and one with a lymphoma; lung adenomas were reported in five treated mice and two controls. In a concurrent experiment in which benzylidene chloride was tested for a shorter duration, a low incidence of skin papillomas was observed. (IARC, 1982). In humans, an excess of respiratory cancer has been reported (six cases in total) in benzoyl chloride manufacturing workers, who were also potentially exposed to benzylidene chloride (IARC, 1982).

3. Evaluation by other organisations

According to IARC, there is *limited evidence* that benzylidene chloride is carcinogenic in experimental animals. The epidemiological data were inadequate to evaluate the carcinogenicity of benzylidene chloride alone, but they provide *limited evidence* that employment in the production of benzoyl chloride and its chlorinated toluene precursors, which involves exposure to benzylidene chloride, represents a carcinogenic risk to man (IARC 1982). In 1999, IARC concluded that combined exposures to alpha-chlorinated toluenes and benzoyl chloride are *probably carcinogenic to humans (Group 2A)* (IARC, 1999).

In their evaluation in 1985, US EPA concluded that the existing data on benzylidene chloride are insufficient for deriving an Acceptable Daily Intake (ADI) or a carcinogenic potency factor (US EPA, 1985).

4. Evaluation

Only very limited data are available regarding the human health effects of benzylidene chloride. These data do not allow determination of a TDI or TCA for benzylidene chloride. However, the available data do indicate that benzylidene chloride has a similar toxic potential as the closely related compound benzyl chloride. As a possible approach the limit values for benzyl chloride can provisionally be adopted for benzylidene chloride. Thus, a provisional oral risk-specific dose (RSD) of one in million per lifetime of 6 ng/kg bw/day and a provisional inhalation risk-specific concentration (RSC) of 28 ng/m^3 are proposed for benzylidene chloride. Considering the small database on benzylidene chloride and the fact that the limit values are based on read-across from benzyl chloride, the reliability of these provisional values is low.

5. Conclusion

Compound	**pRSD$_{oral}$ ***	**pRSC $_{inhalation}$ ***
Benzylidene chloride	6 ng/kg bw/day	28 ng/m^3

* Provisional value based on read-across from benzyl chloride as a structural analogue

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Appendix 5. Detailed aquatic toxicity data for benzylidene chloride

Table A5.1 Acute toxicity data for freshwater species

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T	Hardness CaCO3 [mg/L]	Exp time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria																
Pseudomonas fluorescens		N			99					24 h	EC0		100	3	1,2	IUCLID, Bayer AG
Pisces																
Leuciscus idus		N	S		99.0					48 h	LC0	mortality	50	3	1,3	IUCLID, Bayer AG
Leuciscus idus		N	S		99.0					48 h	LC100	mortality	100	3	1,3	IUCLID, Bayer AG

Notes
1 unknown if closed systems were used
2 according to German test methods (1968)
3 according to German test methods (1979)

Table A5.2 Acute toxicity data for marine species

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T	Salinity [‰]	Exp time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria																
Vibrio fischeri		N	S		99		5-8	15		5 min	EC50	bioluminescence	2.12	2	1,2	Kaiser and Ribo, 1988
Vibrio fischeri		N	S		99		5-8	15		15 min	EC50	bioluminescence	3.44	2	1,2	Kaiser and Ribo, 1988
Vibrio fischeri		N	S		99		5-8	15		30 min	EC50	bioluminescence	5.85	2	1,2	Kaiser and Ribo, 1988
Vibrio fischeri		N	S							30 min	EC50	bioluminescence	4.61	4	1,3	IUCLID, Kaiser et al., 1987
Vibrio fischeri		N	S							30 min	EC50	bioluminescence	32	4	1,4	IUCLID, Steinhauser et al., 1987

Notes
1 not reported whether systems are closed
2 EC50 recalculated from reported log (L/mmol)
3 original reference could not be retrieved
4 reported endpoint cannot be found in cited reference

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