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Environmental risk limits for chlorotoluenes (o-chlorotoluene, m-chlorotoluene, p-chlorotoluene)

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RIVM Report 601782021/2009

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Rapport in het kort

Milieurisiccogrenzen voor chloortoluenen (*o*-chloortolueen, *m*-chloortolueen, *p*-chloortolueen)

Het RIVM heeft milieurisicogrenzen afgeleid voor chloortoluenen in water, grondwater, bodem en lucht. De groep stoffen omvat *o*-chloortolueen, *m*-chloortolueen en *p*-chloorotolueen. Deze stoffen worden gebruikt bij chemische productieprocessen en als oplosmiddel.

Voor deze afleiding zijn actuele ecotoxicologische gegevens gebruikt die zijn gecombineerd met de methodiek die is voorgeschreven door de Europese Kaderrichtlijn Water. De nieuwe ecotoxicologische gegevens laten zien dat de gevoeligheid van het ecosysteem voor chloortoluenen groter is dan voorheen bekend was. Hierdoor zijn de nieuwe milieurisicogrenzen lager dan de eerder afgeleide normen.

Gezien de monitoringsgegevens en de fysisch-chemische eigenschappen van de stoffen worden de nieuwe milieurisicogrenzen naar verwachting niet overschreden. Voor de waterbodem zijn geen milieurisicogrenzen afgeleid want de binding van chloortoluenen aan sediment blijft beneden de grenswaarde. Hierdoor is de blootstelling van waterorganismen aan chloortoluenen via sediment minimaal.

Milieurisicogrenzen zijn maximale concentraties van een stof in het milieu om mens en ecosysteem op verschillende niveaus te beschermen tegen nadelige effecten. Nederland onderscheidt hierbij: een niveau waarbij het risico verwaarloosbaar wordt geacht (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (MTR), het maximaal aanvaardbare niveau voor ecosystemen, specifiek voor kortdurende blootstelling (MAC_{eco}) en tot slot het niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}). De milieurisicogrenzen dienen als advieswaarden voor de Nederlandse Interdepartementale Stuurgroep Stoffen. De stuurgroep stelt de uiteindelijke milieukwaliteitsnormen vast. De overheid hanteert milieukwaliteitsnormen om het nationale stoffenbeleid en de Europese Kaderrichtlijn Water uit te voeren.

Trefwoorden:
milieurisicogrenzen, chloortolueen, *o*-chloortolueen, *m*-chloortolueen, *p*-chloortolueen

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Abstract

Environmental risk limits for chlorotoluenes (*o*-chlorotoluene, *m*-chlorotoluene, *p*-chlorotoluene)

The RIVM has derived environmental risk limits for chlorotoluenes in water, groundwater, soil and air. Current environmental levels of chlorotoluenes are not expected to exceed these limts. This group of substances contains *o*-chlorotoluene, *m*-chlorotoluene and *p*-chlorotoluene. These substances are used as chemical intermediate or as a solvent.

Current ecotoxicological data have been used to derive these values according to methodology as required by the European Water Framework Directive (WFD). The current ecotoxicological data show that the sensitivity of the aquatic ecosystems towards chlorotoluenes is higher than previously known. For this reason, the newly derived environmental risk limits are lower than previously derived limits.

Monitoring data and physico-chemical characteristics of the chlorotoluenes do lead to the expectation that the newly derived environmental risk limits will not be exceeded. No risk limits were derived for the sediment compartment, because sorption to sediment is below the trigger value to derive such risk limits. Exposure of water organisms to chlorotoluenes via the sediment is considered to be negligible.

Environmental risk limits are the maximum allowable concentrations of a substance in the environment to protect humans and the environment for any adverse effect. Four different levels are distinguished: Negligible Concentrations (NC), the concentration at which no harmful effects are to be expected (Maximum Permissible Concentration, MPC), the Maximum Acceptable Concentration for ecosystems specifically for short-term exposure (MAC_{eco}) and a concentration at which serious effects are to be expected (Serious Risk Concentrations, SRC_{eco}). Environmental risk limits form the scientific basis on which the Interdepartmental Steering Committee for Substances sets the environmental quality standards. The government uses these quality standards for carrying out the national policy concerning substances and the European Water Framework Directive.

Key words:
environmental risk limits, chlorotoluene, *o*-chlorotoluene, *m*-chlorotoluene, *p*-chlorotoluene

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Preface

The goal of this report is to derive risk limits that protect both man and the environment. This is done in accordance with the methodology of the Water Framework Directive (WFD). This methodology is incorporated in the Guidance for the derivation of environmental risk limits within the framework of the project 'International and National environmental quality standards for Substances in the environment (INS)' (Van Vlaardingen and Verbruggen, 2007).

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). This advisory group provides a non binding scientific advice on the final draft of a report in order to advise the Dutch Steering Committee for Substances on the scientific merits of the report.

Acknowledgements

Thanks are due to dr. M.P.M. Janssen who is program coordinator for the derivation of Environmental Risk Limits (ERLs) at the RIVM. Ing. P.J.C.M. Janssen (RIVM-Centre for Substances and Integrated Risk Assessment) is thanked for his assistance in the human toxicological part.

The results of the present report have been discussed in the scientific advisory group INS (WK INS). The members of this group are acknowledged for their contribution.

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Contents

Summary

Environmental risk limits are derived using ecotoxicological, physicochemical, and human toxicological data. They represent environmental concentrations of a substance offering different levels of protection to man and ecosystems. It should be noted that the Environmental Risk Limits (ERLs) are scientifically derived values. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have an official status.

In this report, the risk limits Negligible Concentration (NC), Maximum Permissible Concentration (MPC), Maximum Acceptable Concentration for ecosystems (MAC_{eco}), and Serious Risk Concentration for ecosystems (SRC_{eco}) are derived for chlorotoluenes (*o*-chlorotoluene, *m*-chlorotoluene and *p*-chlorotoluene) in water, groundwater, soil and air. No risk limits were derived for the sediment compartment because exposure of sediment is considered negligible. Since not enough data were available for *m*- and *p*-chlorotoluene, the ERLs derived are based on a pooled dataset. They are sum values, so they apply to the total concentration of the three chlorotoluenes discussed in this report.

For the derivation of the MPC and MAC_{eco} for water, the methodology used is in accordance with the Water Framework Directive. This methodology is based on the Technical Guidance Document on risk assessment for new and existing substances and biocides (EC, 2003). For the NC and the SRC_{eco}, the guidance developed for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' was used (Van Vlaardingen and Verbruggen, 2007). An overview of the derived ERLs is given in Table 1.

Table 1. Derived sum MPC, NC, MAC_{eco}, and SRC_{eco} values for *o*-, *m*-, and *p*-chlorotoluene.

ERL	Unit	MPC	NC	MAC_{eco}	SRC_{eco}
Fresh water [a]	$\mu g.L^{-1}$	14	0.14	3.6×10^2	5.2×10^2
Drinking water [b]	$\mu g.L^{-1}$	70	n.a.	n.a.	n.a.
Marine water	$\mu g.L^{-1}$	1.4	0.014	36	5.2×10^2
Soil	$\mu g.kg_{dwt}^{-1}$	4.2×10^2	4.2	n.a.	2.0×10^4
Groundwater	$\mu g.L^{-1}$	14	0.14	n.a.	5.2×10^2
Air	$\mu g.m^{-3}$	7.8×10^2	7.8	n.a.	n.a.

[a] From the $MPC_{eco, water}$, $MPC_{sp, water}$ and $MPC_{hh, food, water}$ the lowest one is selected as the 'overall' MPC_{water}.
[b] The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion. Therefore, the $MPC_{dw, water}$ is presented as a separate value in this report.
n.a. = not applicable.

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1 Introduction

1.1 Background and scope of the report

In this report, environmental risk limits (ERLs) for surface water, groundwater, soil and air are derived for *o*-, *m*- and *p*-chlorotoluene. The derivation is performed within the framework of the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS). The following ERLs are considered:

- Negligible Concentration (NC) – 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 (see next bullet) by a factor of 100.
- Maximum Permissible Concentration (MPC) – 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 death of 10^{-6} per lifetime can be calculated (for genotoxic carcinogenic substances).
- Maximum Acceptable Concentration (MAC_{eco}) – concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Concentration (SRC_{eco}) – concentration at which possibly serious ecotoxicological effects are to be expected.

These ERLs serve as advisory values that are used by the Steering Committee for Substances to set environmental quality standards (EQS) for various policy purposes. EQSs are all legally and non-legally binding standards that are used in Dutch environmental policy.

1.2 Selection of substances

ERLs are derived for *o*-chlorotoluene, *m*-chlorotoluene and *p*-chlorotoluene (Table 2), which were selected by the Dutch government within the framework of 'International and national environmental quality standards for substances in the Netherlands' (INS). The current environmental quality standards for these compounds are based on Van de Plassche et al. (1993). Using a QSAR-approach, they derived MPCs of 0.30, 0.33 and 0.30 $mg.L^{-1}$ for *o*-, *m*- and *p*-chlorotoluene, respectively. The overall MPC_{water} for monochlorotoluenes was set to 0.31 $mg.L^{-1}$, based on total content (310 $\mu g.L^{-1}$). In that report, no ERLs for soil and sediment were derived due to a lack of data.

Table 2. Selected compounds.

Compound	CAS number
o-chlorotoluene	95-49-8
m-chlorotoluene	108-41-8
p-chlorotoluene	106-43-4

1.3 Production and use of chlorotoluenes

Chlorotoluenes are produced by converting toluene with chlorine under moderate temperature and normal pressure in the presence of a catalyst. This gives a crude product with the isomeric ratio of chlorotoluenes depending on temperature and the catalyst. A part of this isomer mixture is processed directly, the other part is used for gaining the isomers by fractional distillation. The produced isomer mixture is processed on-site to cresoles. Cresoles are further used for the production of flame retardants, plasticizers, agrochemicals, material preservatives, thermal oils, fragrances, condenser fluids, and anti-aging agents. The main isomer used individually is *o*-chlorotoluene. *o*-Chlorotoluene is used as an intermediate in the chemical industry and as a solvent for chemical processing as well as a solvent for the formulation of agricultural pesticides. Mixtures of *o*-, *p*- and *m*-chlorotoluene are also used as solvent for herbicides (OECD-SIDS, 2000). The isomeric mixtures produced by Bayer (Germany) contain 40-45% *o*-chlorotoluene and 45-60% *p*-chlorotolunen (IUCLID, 2000) The worldwide production of chlorotoluenes is estimated at 130 000 tonnes per year. The production of *o*-chlorotoluene is about 60 000 – 70 000 tonnes per year (OECD-SIDS, 2000). In Europe, chlorotoluenes are classified as high production volume chemical. The European producers and importers are located in Leverkusen (Germany), Milan (Italy) and Haslemere (UK). There is no production of chlorotoluenes in the Netherlands (ECB website: ecb.jrc.ec.europa.eu/esis/ accessed: 31-10-2008). In the Netherlands, two potential sources for pollution by chlorotoluene utilising industry are identified in the Westerscheld area (VROM, 2004). Chlorotoluenes were also considered relevant for the Rhine area (ICBR, 2007). Since they have not been observed above the detection limit for several years, they are proposed for removal from the Rhine substances list of the International Commission for the Protection of the Rhine (ICBR).

1.4 Status of the results

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 proposed values that do not have an official status.

2 Methods

The methodology for the derivation of ERLs is described in detail by Van Vlaardingen and Verbruggen (2007), further referred to as the 'INS-Guidance'. This guidance is in accordance with the guidance of the Fraunhofer Institute (FHI; Lepper, 2005).

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.

2.1 Data collection

An on-line literature search was performed on TOXLINE (literature from 1985 to 2001) and Current Contents (literature from 1997 to 2007). In addition to this, all references in the RIVM e-tox base and EPA's ECOTOX database were evaluated (an additional 25 references). All toxicity data are reported in the appendices. Studies reported in Van de Plassche et al. (1993) have been reassessed for this report.

2.2 Data evaluation and selection

Substance identification, physico-chemical properties and environmental behaviour was included according to the methods as described in section 2.1 of the INS-Guidance.

Ecotoxicity studies were screened for relevant endpoints (i.e. those endpoints that have consequences at the population level of the test species). All ecotoxicity and bioaccumulation tests were then thoroughly evaluated with respect to the validity (scientific reliability) of the study. A detailed description of the evaluation procedure is given in the INS-Guidance (section 2.2.2 and 2.3.2). In short, the following reliability indices were assigned (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.).'

All available studies were summarised in data-tables, that are included as Annexes 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.

Endpoints with Ri 1 or 2 are accepted as valid, but this does not automatically mean that the endpoint is selected for the derivation of ERLs. The validity scores are assigned on the basis of scientific reliability, but valid endpoints may not be relevant for the purpose of ERL-derivation (e.g. due to inappropriate exposure times or test conditions that are not relevant for the Dutch situation).

After data collection and validation, toxicity data were combined into an aggregated data table with one effect value per species according to section 2.2.6 of the INS-Guidance. When for a species several effect data were available, the geometric mean of multiple values for the same endpoint was calculated where possible. Subsequently, when several endpoints were available for one species, the lowest of these endpoints (per species) is reported in the aggregated data table.

2.3 Specific considerations relating to the test compound

Considering the volatility of the chlorotoluenes the concentration of the compound should be determined during the experiment. Therefore Ri2 is assigned to all studies where the outcome is based on measured concentrations. An exception is made for acute closed static algae tests since these species react to the initial exposure mainly. Also tests with *Vibrio fischeri* are assigned Ri2 because these tests have a very short exposure period.

2.4 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 selection of the final MPC_{water}, some additional comments should be made:

2.4.1 Sum ERLs

Detailed toxicity data for all chlorotoluenes are tabulated in Appendix 2. Complete datasets are not available and when the individual compounds are considered, ERLs cannot be derived for chlorotoluenes. Because the compounds occur in an isomer mixture and toxicity is within the same order of magnitude, derivation of sum-ERLs is considered most appropriate (for further discussion see section 4.2.1). Therefore, all data for the three substances were pooled to derive one set of environmental risk limits which applies to the total concentration of all three chlorotoluenes.

2.4.2 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 INS-Guidance, section 3.1.6 and 3.1.7). According to the proposal for the daughter directive Priority Substances, however, the derivation of the 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 exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion within the framework of the 'AMvB Kwaliteitseisen en Monitoring Water'. No policy decision has been taken yet, and the $MPC_{dw, water}$ is therefore presented as a separate value in this report.

The $MPC_{dw, water}$ is also used to derive the MPC_{gw}. For the derivation of the $MPC_{dw, water}$, a substance specific removal efficiency related to simple water treatment may be needed. Because there is no agreement as yet on how the removal fraction should be calculated, water treatment is not taken into account.

2.4.3 $MAC_{eco, marine}$

In this report, a MAC_{eco} is also derived for the marine environment. The assessment factor for the $MAC_{eco, marine}$ value is based on:

- the assessment factor for the $MAC_{eco, water}$ value when acute toxicity data for at least two specific marine taxa are available, or
- using an additional assessment factor of 5 when acute toxicity data for only one specific marine taxon are available (analogous to the derivation of the MPC according to Van Vlaardingen and Verbruggen, 2007), or
- using an additional assessment factor of 10 when no acute toxicity data are available for specific marine taxa.

If freshwater and marine data sets are not combined the $MAC_{eco, marine}$ is derived on the marine toxicity data using the same additional assessment factors as mentioned above. It has to be noted that this procedure is currently not agreed upon. Therefore, the $MAC_{eco, marine}$ value needs to be re-evaluated once an agreed procedure is available.

3 Substance identification, physico-chemical properties, fate and human toxicology

3.1 *o*-Chlorotoluene

3.1.1 Identity

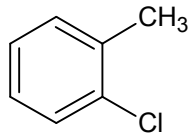

Figure 1. Structural formula of *o*-chlorotoluene.

Table 3. Identification of *o*-chlorotoluene.

Parameter	Value
Common/trivial/other name	*o*-chlorotoluene, 2-chlorotoluene
Chemical name	1-chloro-2-methylbenzene
CAS number	95-49-8
EC number	202-424-3
SMILES code	c(c(ccc1)Cl)(c1)C

3.1.2 Physico-chemical properties

Table 4. Physico-chemical properties of *o*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	126.6		
Water solubility	[mg.L^{-1}]	**117**	25°C, shake flask-GC/FID	Ma et al., 2001
		47	20°C, method unpublished	BUA 038, 1989, orig. ref.: Bayer, 1987
log K_{OW}	[-]	2.95		Karickhoff et al., 2007
		3.18	EPIwin	US EPA, 2007
		3.4	HPLC-k'	Mackay et al., 2006
		3.42	MlogP	BioByte, 2006
		3.42	Shake flask	Mackay et al., 2006
		3.52	HPLC-RT, recommended	Mackay et al., 2006
log K_{OC}	log [L.kg^{-1}]	2.65	EPIwin	US EPA, 2007
		2.87	QSAR	Van Vlaardingen and Verbruggen, 2007
Vapour pressure	[Pa]	487	25°C, Interpol.-Antoine equation	Mackay et al., 2006, orig. ref.: Stuckey & Saylor et al., 1940
		485	25°C, Interpol.-Antoine equation	Mackay et al., 2006, orig. ref.: Dean, 1985, 1992

Parameter	Unit	Value	Remark	Reference
		486	geometric mean of Interpol. Antoine equation for 25°C given above	
		309	EPIwin, 25°C	US EPA, 2007
		427	25°C	Karickhoff et al., 2007
Melting point	[°C]	-35.8		Mackay et al., 2006
		-35.4		BUA 038, 1989, orig. ref.: Rathjen, 1975
Boiling point	[°C]	159		Mackay et al., 2006
		159		BUA 038, 1989, orig. ref.: Rathjen, 1975
Henry's law const.	[$Pa.m^3.mol^{-1}$]	**362**	25°C, van 't Hoff equation	Staudinger and Roberts, 2001
		970	20°C	BUA 038, 1989, orig. ref.: Bayer, 1987
		447	EPIwin, bond method	US EPA, 2007
		494	EPIwin, group method	US EPA, 2007
		273		Karickhoff et al., 2007

3.1.3 Behaviour in the environment

Hydrolysis of *o*-chlorotoluene does not occur under environmentally relevant conditions. In water, volatilisation is the main removal process. EPIwin (US EPA, 2007) indicates *o*-chlorotoluene as not readily biodegradable.

3.1.4 Bioconcentration and biomagnification

There are no experimental bioaccumulation data for *o*-chlorotoluene. The calculated bioconcentration factor is given in Table 5.

Table 5. Overview of bioaccumulation data for *o*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[$L.kg^{-1}$]	56.53	EPIwin	US EPA, 2007
		161	QSAR	Van Vlaardingen and Verbruggen, 2007
BMF	[$kg.kg^{-1}$]	1	Default value	

3.1.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases are assigned to *o*-chlorotoluene: R20, R51/53, *o*-chlorotoluene is not classified as being a carcinogen.

A NOEL of 20 $mg.kg_{bw}^{-1}$ for rat and dog is available (OECD-SIDS, 2000). The US-EPA has derived a Reference Dose (RfD) of 0.02 $mg.kg_{bw}^{-1}day^{-1}$ based on the NOEL for rats with an AF of 1000. RIVM has also derived a TDI of 0.02 $mg.kg_{bw}^{-1}day^{-1}$ in 1996 (Slooff et al., 1996). This value of 0.02 $mg.kg_{bw}^{-1}day^{-1}$ will be used as TDI in this report. A TCA of 775 $\mu g.m^{-3}$ was derived by Rademaker et al. (1993).

3.2 *m*-Chlorotoluene

3.2.1 Identity

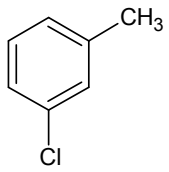

Figure 2. Structural formula of *m*-chlorotoluene.

Table 6. Identification of *m*-chlorotoluene.

Parameter	Value
Common/trivial/other name	*m*-chlorotoluene, 3-chlorotoluene
Chemical name	1-chloro-3-methylbenzene
CAS number	108-41-8
EC number	203-580-5
SMILES code	c(cccc1Cl)(c1)C

3.2.2 Physico-chemical properties

Table 7. Physico-chemical properties of *m*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	126.6		
Water solubility	[mg.L^{-1}]	**117**	25°C, shake flask - GC/FID	Ma et al., 2001
		57	20°C, method unpublished	BUA 038, 1989, orig. ref.: Bayer, 1987
pK_a	[-]			
log K_{OW}	[-]	3.0		Karickhoff et al., 2007
		3.18	EPIwin	US EPA, 2007
		3.28	Shake flask, recommended	Mackay et al., 2006
		3.28	MlogP	BioByte, 2006
		3.4	HPLC-k' correlation	Mackay et al., 2006
log K_{OC}	log [L.kg^{-1}]	2.64	EPIwin	US EPA, 2007
		2.76	QSAR	Van Vlaardingen and Verbruggen, 2007
Vapour pressure	[Pa]	**418**	25°C, Interpol.-Antoine eq.	Mackay et al., 2006
		309	EPIwin	US EPA, 2007
		449		Karickhoff et al., 2007
Melting point	[°C]	-47.8		Mackay et al., 2006
		-48.7		BUA 038, 1989, orig. ref.: Rathjen, 1975
Boiling point	[°C]	161.8		Mackay et al., 2006
		161.2		BUA 038, 1989, orig. ref.: Rathjen, 1975
Henry's law const.	[Pa.m^3.mol^{-1}]	447	EPIwin: bond method	US EPA, 2007

Parameter	Unit	Value	Remark	Reference
		496	EPIwin: group method	US EPA, 2007
		314		Karickhoff et al., 2007
		800	20°C	BUA 038, 1989, orig. ref.: Bayer, 1987
		452	MW x VP / WS	

3.2.3 Behaviour in the environment

Hydrolysis of *m*-chlorotholuene does not occur under environmentally relevant conditions. In water, volatilisation is the main removal process. EPIwin (US EPA, 2007) indicates *m*-chlorotoluene as not readily biodegradable.

3.2.4 Bioconcentration and biomagnification

There are no experimental bioaccumulation data for *m*-chlorotoluene. The calculated bioconcentration factor is given in Table 8.

Table 8. Overview of bioaccumulation data for *m*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[$L.kg^{-1}$]	56.53	EPIwin	US EPA, 2007
		122	QSAR	Van Vlaardingen and Verbruggen, 2007
BMF	[$kg.kg^{-1}$]	1	Default value	

3.2.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases are assigned to m-chlorotoluene: R20, R51/53, *m*-chlorotoluene is not classified as being a carcinogen. For *m*-chlorotoluene no TDI or TCA is available.

3.3 *p*-Chlorotoluene

3.3.1 Identity

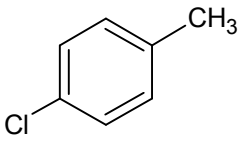

Figure 3. Structural formula of *p*-chlorotoluene.

Table 9. Identification of *p*-chlorotoluene.

Parameter	Value
Common/trivial/other name	*p*-chlorotoluene, 4-chlorotoluene
Chemical name	1-chloro-4-methylbenzene
CAS number	106-43-4
EC number	203-397-0
SMILES code	c(ccc(c1)Cl)(c1)C

3.3.2 Physico-chemical properties

Table 10. Physico-chemical properties of *p*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	126.6		
Water solubility	[mg.L^{-1}]	**123**	Shake flask-GC/FID	Mackay et al., 2006
		40	20°C, method unpublished	BUA 038, 1989, orig. ref.: Bayer, 1987
pK_a	[-]			
log K_{OW}	[-]	3.0		Karickhoff et al., 2007
		3.18	EPIwin	US EPA, 2007
		3.3	shake flask	Mackay et al., 2006
		3.33	shake flask, recommended	Mackay et al., 2006
		3.33	MlogP	BioByte, 2006
		3.4	HPLC-k' correlation	Mackay et al., 2006
		3.42	HPLC-RT correlation	Mackay et al., 2006
log K_{OC}	log [L.kg^{-1}]	2.64	EPIwin	US EPA, 2007
		2.80	QSAR	Van Vlaardingen and Verbruggen, 2007
Vapour pressure	[Pa]	422	25°C, Interpol.-Antoine eq.	Mackay et al., 2006
		471.6	25°C, Interpol.-Antoine eq.	Mackay et al., 2006
		446	geometric mean of Interpol. Antoine values presented above for 25°C	
		309	EPIwin	US EPA, 2007
		419		Karickhoff et al., 2007
Melting point	[°C]	7.5		Mackay et al., 2006
		7.6		BUA 038, 1989, orig. ref.: Rathjen, 1975
Boiling point	[°C]	162.4		Mackay et al., 2006
		161.5	at 1013hPa	BUA 038, 1989, orig. ref.: Rathjen, 1975
Henry's law const.	[Pa.m^3.mol^{-1}]	412.4	calculated	Mackay et al., 2006
		980	20°C	BUA 038, 1989, orig. ref.: Bayer, 1987
		447	EPIwin, bond method	US EPA, 2007
		494	EPIwin, group method	US EPA, 2007
		299		Karickhoff et al., 2007
		459	MW x VP / WS	

3.3.3 Behaviour in the environment

Hydrolysis of *p*-chlorotholuene does not occur under environmentally relevant conditions. In water, volatilisation is the main removal process. EPIwin (US EPA, 2007) indicates *p*-chlorotoluene as not readily biodegradable.

3.3.4 Bioconcentration and biomagnification

There are no experimental bioaccumulation data for *p*-chlorotoluene. The calculated bioconcentration factor is given in Table 11.

Table 11. Overview of bioaccumulation data for *p*-chlorotoluene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[$L.kg^{-1}$]	56.53	EPIwin, QSAR	US EPA, 2007
		135	QSAR	Van Vlaardingen and Verbruggen, 2007
BMF	[$kg.kg^{-1}$]	1	Default value	

3.3.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases are assigned to *p*-chlorotoluene: R20, R51/53, *p*-chlorotoluene is not classified as being a carcinogen. For *p*-chlorotoluene no TDI or TCA is available.

4 Derivation of environmental risk limits

4.1 Trigger values

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

Table 12. *o*-Chlorotoluene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.87	log [L.kg^{-1}]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.1.2
BCF	161	[L.kg^{-1}]		3.1.4
BMF	1	[kg.kg^{-1}]		3.1.4
Log K_{OW}	3.42	[-]		3.1.2
R-phrases	20, 51/53	[-]		3.1.5
A1 value	-	[µg.L^{-1}]		
DW standard	-	[µg .L^{-1}]		

[1] $f_{OC,susp}$ = 0.1 $kg_{OC}.kg_{solid}^{-1}$ (EC, 2003).

- *o*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; derivation of $MPC_{sediment}$ is not triggered.
- *o*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- *o*-chlorotoluene has a log $K_{ow} >$ 3; assessment of secondary poisoning is triggered.
- *o*-chlorotoluene has no R classification for which an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) needs to be derived.

Table 13. *m*-Chlorotoluene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.76	log [L.kg^{-1}]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.2.2
BCF	122	[L.kg^{-1}]		3.2.4
BMF	1	[kg.kg^{-1}]		3.2.4
Log K_{OW}	3.28	[-]		3.2.2
R-phrases	20, 51/53	[-]		3.2.5
A1 value	-	[µg.L^{-1}]		
DW standard	-	[µg.L^{-1}]		

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

- *m*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; derivation of $MPC_{sediment}$ is not triggered.
- *m*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- *m*-chlorotoluene has a log $K_{ow} >$ 3; assessment of secondary poisoning is triggered.
- *m*-chlorotoluene has no R classification for which an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) needs to be derived.

Table 14. *p*-Chlorotoluene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.80	log [L.kg^{-1}]	$K_{OC} \times f_{OC,susp}$[1]	K_{OC}: 3.3.2
BCF	135	[L.kg^{-1}]		3.3.4
BMF	1	[kg.kg^{-1}]		3.3.4
Log K_{OW}	3.33	[-]		3.3.2
R-phrases	20, 51/53	[-]		3.3.5
A1 value	-	[µg.L^{-1}]		
DW standard	-	[µg.L^{-1}]		

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

- *p*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; derivation of $MPC_{sediment}$ is not triggered.
- *p*-chlorotoluene has a log $K_{p,\ susp\text{-}water} <$ 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- *p*-chlorotoluene has a log $K_{ow} >$ 3; assessment of secondary poisoning is triggered.
- *p*-chlorotoluene has no R classification for which an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) needs to be derived.

4.2 Aquatic compartment

4.2.1 Aquatic toxicity data

Detailed toxicity data for all chlorotoluenes are tabulated in Appendix 2. No complete basesets (algae, Daphnia, fish) are available for the respective isomers. Considering the datasets, ERLs cannot be derived for the individual compounds. Based on the valid studies, the data indicate, however, that there are no large differences in toxicity between the three substances. For example, for the crustacean, *o*-chlorotoluene has a NOEC value of 0.14 mg.L^{-1} and *p*-chlorotoluene has NOEC values of 0.32 mg.L^{-1}, 0.56 mg.L^{-1} and 1 mg.L^{-1}. Also, the difference between log K_{ow} of the three isomers is at most 0.14. Assuming that the mechanism of toxicity is narcosis, this small difference in log K_{ow} supports the observation of similar toxicity for the three isomers. It should be noticed that there is very little data for *m*-chlorotoluene and therefore we cannot be absolutely certain that the toxicity of this isomer is indeed similar to that of the other two isomers. *m*-Chlorotoluene is however produced in minor amounts as compared to the other two isomers. As indicated in section 1.3, the isomeric mixtures produced consists mainly of *o*-, and *p*-chlorotoluene and the concentration of *m*-chlorotoluene in the environment is therefore also expected to be much lower than that of the other two isomers. If the toxicity of the *m*-isomer would be higher as compared to the other two isomers, this would then be of limited influence on the total toxicity of the isomeric mixture in the environment. Therefore it is considered justified that all data for the three substances are pooled to derive one set of environmental risk limits which applies to the total concentration of the three isomers. An overview of the selected freshwater toxicity data for the chlorotoluenes is given in Table 15. Only limited reliable marine toxicity data have been collected (Table 16). Unbounded values are also presented in Table 15. These values are only indicative of relative insensitivity of a tested taxon and are not used for derivation of the ERLs.

Table 15. Chlorotoluene: selected freshwater toxicity data for ERL derivation.

Chronic[a]		Acute[a]	
Taxonomic group	**NOEC/EC10 (mg.L^{-1})**	**Taxonomic group**	**L(E)C50 (mg.L^{-1})**
Algae		Algae	
Scenedesmus subspicatus	>100	*Scenedesmus subspicatus*	>100
Crustacea		Crustacea	
Daphnia magna	**0.14** [b]	*Daphnia magna*	**3.6** [c]
		Ceriodaphnia cf. *dubia*	16.5
Pisces			
Danio rerio	1.9		

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.
[b] Lowest 21 d NOEC
[c] Lowest 48 h LC50

Table 16 Chlorotoluene: selected marine toxicity data for ERL derivation.

Chronic[a]		Acute[a]	
Taxonomic group	**NOEC/EC10 (mg.L^{-1})**	**Taxonomic group**	**L(E)C50 (mg.L^{-1})**
		Bacteria	
		Vibrio fischeri	5.7 [a]

[a] Geometric mean of 6.34, 4.92 and 5.92 mg.L^{-1}.

4.2.2 Treatment of fresh- and saltwater toxicity data

Only limited reliable marine data are available therefore freshwater and marine data are pooled for ERL derivation.

4.2.3 Mesocosm studies

No mesocosm studies are available for chlorotoluenes.

4.2.4 Derivation of MPC_{water} and MPC_{marine}

4.2.4.1 $MPC_{eco, water}$ and $MPC_{eco, marine}$

There is no complete reliable base set of L/EC50 values, but the absence of an acute LC50 for fish is compensated for by the chronic NOEC. The trophic level of the lowest LC50 is included in the trophic levels of the NOEC/EC10s and there are three NOECs representing three trophic levels (algae, *Daphnia* and fish). Therefore an assessment factor of 10 is applied to the lowest value of 0.14 mg.L^{-1} for *Daphnia magna*. The $MPC_{eco, water}$ is: 0.14 / 10 = 0.014 mg.L^{-1} = 14 µg.L^{-1}

Based on the same arguments as for the $MPC_{eco, water}$, the $MPC_{eco, marine}$ is derived with a factor of 100 on the NOEC of 0.14 mg.L^{-1} for *D. magna*. There are no additional marine species to reduce the assessment factor, because *Vibrio fischeri* has the same life form and feeding strategy as freshwater bacteria. Therefore the $MPC_{eco, marine}$ is 1.4 µg.L^{-1}.

4.2.4.2 $MPC_{sp, water}$ and $MPC_{sp, marine}$

The chlorotoluenes have log K_{ow} values > 3, thus assessment of secondary poisoning is triggered.

To derive the $MPC_{sp, water}$ the NOEL of 20 mg.kg$_{bw}^{-1}$.day^{-1} for *o*-chlorotoluene as given in section 3.1.5 for a three months repeated dose study can be converted into a NOEC using a conversion factor. Since

no age of the animals was given, the lower conversion factor of 10 is used as a worst case scenario. This approach gives a NOEC of 200 mg.kg_{food}. This NOEC can be extrapolated to an $MPC_{oral, mammal}$ using an assessment factor of 90 for a three months study: 200 / 90 = 2.22 mg.kg_{food}^{-1}. With the BCF of 161 L.kg^{-1} and BMF_1 of 1 for *o*-chlorotoluene, the final $MPC_{sp, water}$ is: 2.22 / (161 * 1) = 0.014 mg.L^{-1} = 14 µg.L^{-1}.

The $MPC_{sp, marine}$ is derived with an extra BMF_2. Since the log Kow is lower than 4.5 the BMF_2 is 1. Therefore the $MPC_{sp, marine}$ is equal to the $MPC_{sp, water}$: 14 µg.L^{-1}.

4.2.4.3 $MPC_{hh\ food, water}$

Derivation of $MPC_{hh\ food, water}$ for the chlorotoluenes is not triggered (Table 12, Table 13, and Table 14).

4.2.4.4 Selection of the MPC_{water} and MPC_{marine}

The $MPC_{sp, water}$ and the $MPC_{eco, water}$ have the same value, therefore, the MPC_{water} is 14 µg.L^{-1}
The lowest MPC_{marine} is the $MPC_{eco, marine}$: 1.4 µg.L^{-1}

4.2.5 $MPC_{dw, water}$

No A1 value or DW standard are available for the chlorotoluenes. With the TDI for *o*-chlorotoluene of 0.02 mg.$kg_{bw}^{-1}day^{-1}$ an $MPC_{dw, water, provisional}$ can be calculated with the following formula: $MPC_{dw, water, provisional} = 0.1.TL_{hh}.BW / Uptake_{dw}$ where the TL_{hh} is the TDI, BW is a body weight of 70 kg, and $uptake_{dw}$ is a daily uptake of 2 L. The $MPC_{dw, water, provisional}$ becomes: 0.1 * 0.02 * 70 / 2 = 0.07 mg.L^{-1} = 70 µg.L^{-1}.

4.2.6 Derivation of MAC_{eco}

The MAC_{eco} is based on the lowest $L(E)C_{50}$ value available. Assuming that the chronic NOEC for fish is indicative that fish are not the most sensitive species group, there is a complete base set, a known mode of action and the most sensitive species is included in the dataset. Therefore, an assessment factor of 10 is applied. It should also be noted that the acute to chronic ratio of 26 for *Daphnia* is quite high. There are currently no data to further analyse this observation. The MAC_{eco} is: 3.6 mg.L^{-1}/10 = 0.36 mg.L^{-1} = 360 µg.L^{-1}.

The $MAC_{eco, marine}$ is set a factor of 10 lower than the $MAC_{eco, water}$ because there are no additional marine species to reduce the assessment factor. *Vibrio fischeri* has the same life form and feeding strategy as freshwater bacteria and is therefore not considered as an additional marine species. The $MAC_{eco, marine}$ is 36 µg.L^{-1}.

4.2.7 Derivation of NC

The NC_{water} is set a factor of 100 lower than the MPC_{water}: 0.14 µg.L^{-1}.
The NC_{marine} is: 0.014 µg.L^{-1}.

4.2.8 Derivation of $SRC_{eco, water}$

For calculation of the $SRC_{eco, water}$, the geometric mean of the acute and chronic water toxicity data in Table 15 and 16 has been calculated. Unbounded values (<) have not been used for this calculation. The geometric mean of the acute data divided by 10 is 0.70 mg.L^{-1} which is higher than the geometric mean of the chronic data of 0.52 mg.L^{-1}. Therefore, the $SRC_{eco, water}$ is 0.52 mg.L^{-1} = 5.2 x 10^2 µg.L^{-1}.
The $SRC_{eco, water}$ is valid for the freshwater and the marine environment.

4.3 Sediment

The log $K_{p, susp\text{-}water}$ values of the chlorotoluenes are below the trigger value of 3, therefore, ERLs are not derived for sediment.

4.4 Soil

4.4.1 Soil toxicity data

No suitable experimental data on toxicity to soil organisms are available for the chlorotoluenes.

4.4.2 Derivation of MPC_{soil}

4.4.2.1 $MPC_{eco, soil}$

The $MPC_{eco, soil}$ is calculated from the $MPC_{eco, water}$ using the equilibrium partitioning method (van Vlaardingen and Verbruggen, 2007). For this calculation the geometric mean of the log K_{oc} for *o*-, *m*-, and *p*-chlorotoluene is used (2.81). For the Henry constant, the value of 362 $Pa.m^3.mol^{-1}$ is selected since this is the only experimentally derived value. The calculated $MPC_{eco, soil}$ is 0.54 $mg.kg_{dwt}^{-1}$ = 5.4 x 10^2 $\mu g.kg_{dwt}^{-1}$, based on Dutch standard soil.

4.4.2.2 $MPC_{human, soil}$

The $MPC_{human, soil}$ is based on the TDI of 0.02 $mg.kg_{bw}^{-1}$ for *o*-chlorotoluene (see section 3.1.5). Since the TDI is for *o*-chlorotoluene, the physico-chemical parameters for *o*-chlortoluene have been used for this calculation. Specific human intake routes are allowed to contribute to 10% of the human toxicological threshold limit. Four different routes contributing to human exposure have been considered: consumption of leafy crops, root crops, mild and meat (see INS-guidance section 3.3.6). Uptake via root crops was determined to be the critical route. The $MPC_{human, soil}$ is calculated to be 0.42 $mg.kg_{dwt}^{-1}$ = 4.2 x 10^2 $\mu g.kg_{dwt}^{-1}$, based on Dutch standard soil.

4.4.2.3 Selection of the MPC_{soil}

The lowest MPC_{soil} is the $MPC_{human, soil}$: 0.42 $mg.kg_{dwt}^{-1}$ $_{Dutch\ standard\ soil}$. Thus the MPC_{soil} is 0.42 $mg.kg^{-1}$.

4.4.3 Derivation of NC_{soil}

The NC is set a factor of 100 lower than the MPC. The NC_{soil} is 4.2 $\mu g.kg_{dwt}^{-1}$ for Dutch standard soil.

4.4.4 Derivation of $SRC_{eco, soil}$

Since no toxicity data are available for the soil compartment the SRC_{eco}, soil has been calculated from the $SRC_{eco, water}$ using equilibrium partitioning. The $SRC_{eco, soil}$ is 20 $mg.kg_{dwt}^{-1}$.

4.5 Groundwater

4.5.1 Derivation of MPC_{gw}

4.5.1.1 $MPC_{eco, gw}$

Since groundwater-specific ecotoxicological information is absent, the derived ERLs for surface water based on ecotoxicological data are taken as substitute. Thus, $MPC_{eco, gw} = MPC_{eco, water} = 14\ \mu g.L^{-1}$.

4.5.1.2 $MPC_{human, gw}$

The $MPC_{dw,water, provisional}$ is 0.07 $mg.L^{-1}$. This value is lower than the $MPC_{eco, gw}$, therefore an $MPC_{human, gw}$ should be derived from the $MPC_{dw,water, provisional}$. As described in section 2.2 water treatment is currently not taken into account. Therefore the $MPC_{human, gw} = MPC_{dw, water} = MPC_{dw,water, provisional}$: 0.07 $mg.L^{-1}$ = 70 $mg.L^{-1}$.

4.5.1.3 Selection of the MPC_{gw}

The final MPC_{gw} is the lowest MPC_{gw} derived, the $MPC_{eco, gw}$ of 14 $\mu g.L^{-1}$.

4.5.2 Derivation of NC_{gw}

The NC is set a factor 100 lower than the MPC_{gw}: 0.14 $\mu g.L^{-1}$.

4.5.3 Derivation of $SRC_{eco, gw}$

The $SRC_{eco, gw}$ is set equal to the $SRC_{eco, water}$: 0.52 $mg.L^{-1}$ = 5.2 x 10^2 $\mu g.L^{-1}$.

4.6 Air

4.6.1 Derivation of $MPC_{eco, air}$

Since no data on the ecotoxicity of monochlorobenzenes are available, no $MPC_{eco, air}$ can be derived.

4.6.2 Derivation of $MPC_{human, air}$

The $MPC_{human, air}$ is set at the same value as the TCA derived by Rademaker et al. (1993): 775 $\mu g.m^{-3}$.

4.6.3 Selection of MPC_{air}

The only available value of the routes included is the $MPC_{human, air}$ (775 $\mu g.m^{-3}$).
Therefore, the MPC_{air} for the chlorotoluenes is 775 $\mu g.m^{-3}$ = 7.8 x 10^2 $\mu g.m^{-3}$.

4.6.4 Derivation of NC_{air}

The MPC_{air} divided by 100 is the NC_{air}: 7.8 $\mu g.m^{-3}$.

4.7 Comparison of the derived ERLs with monitoring data

Monitoring data for *o*-chlorotoluene presented by the Dutch Association of River Water Companies (RIWA; www.riwa.org) as well as by the Dutch Ministry of Transport, Public Works and Water

Management (VenW; www.waterstat.nl) do not show any occasion where the concentration of *o*-chlorotoluene exceeded the detection level of 0.01-0.03 $\mu g.L^{-1}$ over the years 2001 – 2007. For the other chlorotoluenes, no monitoring data are available. On the basis of the data for *o*-chlorotoluene it can be concluded that the ERLs derived in this report, which are all higher than the detection limit, will most likely not be exceeded either.

5 Conclusions

In this report, the risk limits Negligible Concentration (NC), Maximum Permissible Concentration (MPC), Maximum Acceptable Concentration for ecosystems (MAC_{eco}), and Serious Risk Concentration for ecosystems (SRC_{eco}) are derived for the total of *o*-chlorotoluene, *m*-chlorotoluene and *p*-chlorotoluene in water, groundwater, soil and air. No risk limits were derived for the sediment compartment because the trigger to derive such limits is not reached.

The ERLs derived, are based on a pooled dataset and, since they are sum values, apply to the total of chlorotoluenes discussed in this report. The ERLs were obtained are summarised in the table below.

Table 17. Derived sum MPC, NC, MAC_{eco}, and SRC_{eco} values for *o*-, *m*-, and *p*-chlorotoluene.

ERL	Unit	MPC	NC	MAC_{eco}	SRC_{eco}
Fresh water [a]	$\mu g.L^{-1}$	14	0.14	3.6×10^2	5.2×10^2
Drinking water [b]	$\mu g.L^{-1}$	70	n.a.	n.a.	n.a.
Marine water	$\mu g.L^{-1}$	1.4	0.014	36	5.2×10^2
Soil	$\mu g.kg_{dwt}^{-1}$	4.2×10^2	4.2	n.a.	2.0×10^4
Groundwater	$\mu g.L^{-1}$	14	0.14	n.a.	5.2×10^2
Air	$\mu g.m^{-3}$	7.8×10^2	7.8	n.a.	n.a.

[a] From the $MPC_{eco, water}$, $MPC_{sp, water}$ and $MPC_{hh, food, water}$ the lowest one is selected as the 'overall' MPC_{water}.
[b] The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion. Therefore, the $MPC_{dw, water}$ is presented as a separate value in this report.
n.a. = not applicable.

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Appendix 1. Detailed aquatic toxicity data

Table A1.1. Acute toxicity of *o*-chlorotoluene to freshwater organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Hardness $CaCO_3$ [$mg.L^{-1}$]	Exp time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Ri	Notes	Reference
Algae															
Scenedesmus subspicatus	strain 8681 SAG, 10000/ml	N	Sc		am	8	24		72h	EC50	growth	>100	2	1	Kühn and Pattard, 1990
Crustacea															
Daphnia magna	<24 h, 0.315-0.630 mm	N	S		tw	7.6-7.7	20-22	286	24 h	EC50	immobility	74	3	4	Bringmann and Kühn, 1977b
Daphnia magna	<24 h, Strauss, IRCHA	N	S		am	8.0±0.2	20	250.2	24 h	EC50	immobility	41	3	4	Bringmann and Kühn, 1982
Daphnia magna	<24 h, IRCHA	N	Sc	-	am	8.0±0.2	25±1	250	24 h	LC50	mortality	20	3	2	Kühn et al., 1989
Daphnia magna	<24 h, 0.315-0.630 mm	N	S		tw	7.6-7.7	20-22	286	24 h	EC0	immobility	46	3	4	Bringmann and Kühn, 1977b
Daphnia magna	<24 h, Strauss, IRCHA	N	S		am	8.0±0.2	20	250.2	24 h	EC0	immobility	19	3	4	Bringmann and Kühn, 1982
Daphnia magna	<24 h, IRCHA	N	Sc	-	am	8.0±0.2	25±1	250	24 h	LC0	mortality	9	3	2	Kühn et al., 1989
Pisces															
Leuciscus idus melanotus		N	S	-	tw	7--8	20±1	255	48 h	LC50	mortality	78	3	3,4	Juhnke and Lüdemann, 1978
Leuciscus idus melanotus		N	S	-	tw	7--8	20±1	255	48 h	LC0	mortality	11	3	3,4	Juhnke and Lüdemann, 1978

1 solubility limit

2 photoperiod 9:15 light:dark with fluorescent light

3 test according to Mann, 1976

4 static test, not closed and not measured

Table A1.2. Acute toxicity of *m*-chlorotoluene to freshwater organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Hardness $CaCO_3$ [$mg.L^{-1}$]	Exp time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Ri	Notes	Reference
Pisces															
Poecilia reticulata	2-3 month old	N	R		am		22	25	7 d	LC50	mortality	18	3	1	Könemann, 1981

1 covered with glass

Table A1.3. Acute toxicity of *p*-chlorotoluene to freshwater organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Hardness $CaCO_3$ [$mg.L^{-1}$[	Exp time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Ri	Notes	Reference
Crustacea															
Daphnia magna	< 48 h	Y	S		am		22±1	100	48 h	EC50	immobility	3.6	2	1	Hermens et al., 1984
Daphnia magna									48 h	EC50	immobility	2.5	4	2	Dearden et al., 2000
Ceriodaphnia cf. *dubia*	< 24 h	Y	Sc	>97%		7.7	23±1	65.2	48 h	EC50	immobility	16.5	2	4	Rose et al., 1998
Daphnia carinata	< 24 h	Y	S				20±1		48 h	EC50	immobility	1.11	4	2,4	Khalil, 1998 in Warne, 1999
Pisces															
Pimephales promelas										LC50	mortality	5.9	4*	2	Dearden et al., 2000
Poecilia reticulata	2-3 month old	N	R		am		22	25	14 d	LC50	mortality	5.9	3	3	Könemann, 1981
Pimephales promelas									7-14 d	LC50	mortality	5.9	4*	2	Zhao et al., 1993

1 test according to NEN 6501. 6502

2 cited in reference

3 covered with glass

4 value based on measured concentrations

Table A1.4. Acute toxicity of *o*-chlorotoluene to marine organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temperature [°C]	Salinity [‰]	Exp time	Criterion	Test endpoint	Value [mg.L^{-1}]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri									30 min	EC50	bioluminescense	4.7	2	1	Sixt et al., 1995
Vibrio fischeri			S		am	5-8	20		5 min	EC50	bioluminescense	5.92	2	1,2	Casseru, 1985 in Kaiser and Ribo, 1988
Vibrio fischeri			S		am	5-8	20		15 min	EC50	bioluminescense	6.06	2	1,2	Casseru, 1985 in Kaiser and Ribo, 1988
Crustacea															
Nitocra spinipes		N	S		nw	7.8	10 or 21	7	96h	LC50		45	3	3,4	Bengtsson and Tarkpea, 1983
Pisces															
Alburnus alburnus		N	S		nw	7.8	20-22	7	96h	LC50		7.8	3	4	Bengtsson and Tarkpea, 1983

1 cited in reference

2 freshly reconstituted bacterial medium

3 temperature not clear in description

4 static test, not closed and not measured

Table A1.5. Acute toxicity of *m*-chlorotoluene to marine organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temperature [°C]	Salinity [‰]	Exp time	Criterion	Test endpoint	Value [mg.L^{-1}]	Ri	Notes	Reference
Crustacea															
Nitocra spinipes		N	S		nw (filtered)	7.8	10 or 21	7	96h	LC50		25	3	1,2	Bengtsson and Tarkpea, 1983

1 temperature not clear in description

2 static test, not closed and not measured

Table A1.6. Acute toxicity of *p*-chlorotoluene to marine organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Salinity [‰]	Exp time	Criterion	Test endpoint	Value [mg.L^{-1}]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri									30 min	EC50	bioluminescense	6.5	2	1	Sixt et al., 1995
Vibrio fischeri		N	S				20		15 min	EC50	bioluminescense	17	2	4	Zhao et al., 1993
Vibrio fischeri			S		am	5-8	20		5 min	EC50	bioluminescense	6.34	2	1,2	Casseru, 1985 in Kaiser and Ribo, 1988
Vibrio fischeri			S		am	5-8	20		15 min	EC50	bioluminescense	7.28	2	1,2	Casseru, 1985 in Kaiser and Ribo, 1988
Vibrio fischeri			S		am	5-8	15		5 min	EC50	bioluminescense	4.92	2	1	Kaiser et al., 1985, in Kaiser and Ribo, 1988
Vibrio fischeri			S		am	5-8	15		15 min	EC50	bioluminescense	5.79	2	1	Kaiser et al., 1985, in Kaiser and Ribo, 1988
Vibrio fischeri			S		am	5-8	15		30 min	EC50	bioluminescense	7.28	2	1	Kaiser et al., 1985, in Kaiser and Ribo, 1988
Crustacea															
Nitocra spinipes		N	S		nw (filtered)	7.8	10 or 21	7	96h	LC50		15	3	3,4	Bengtsson and Tarkpea, 1983

1 cited in reference

2 freshly reconstituted bacterial medium

3 temperature not clear in description

4 static test, not closed and not measured

Table A1.7. Chronic toxicity of *o*-chlorotoluene to freshwater organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Hardness $CaCO_3$ [$mg.L^{-1}$]	Exp time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Ri	Notes	Reference
Bacteria															
Pseudomonas putida		N	Sc		am	7.0	25	81.2	16 h	NOEC	growth	15	3	1,2,9,10	Bringmann and Kühn, 1977a, 1979, 1980b
Cyanophyta															
Microcystis aeruginosa		N	Sc		am	7.0	27	55	8 d	NOEC	growth	31	3	1,2,3,9,10	Bringmann and Kühn, 1978a,b
Protozoa															
Chilomonas paramaecium		N	Sc		am	6.9	20	74.6	48 h	NOEC	growth	>40	3	1,4,10	Bringmann et al., 1980
Entosiphon sulcatum	Stein	N	Sc		am	6.9	25	75.1	72 h	NOEC	growth	>80	3	1,4,10	Bringmann, 1978, Bringmann and Kühn, 1979, 1980b
Uronema parduczi	Chatton-Lwoff	N	Sc		am	6.9	25	75.1	20 h	NOEC	growth	>80	3	1,4,10	Bringmann and Kühn, 1980a
Algae															
Scenedesmus quadricauda		N	Sc		am	7.0	27	55	8 d	NOEC	growth	>100	3	1,3,10	Bringmann and Kühn, 1977a, 1978a,b, 1979, 1980b
Scenedesmus subspicatus		N	Sc		am	7.7-9.3	24		72h	EC10	growth	>100	2		Kuhn and Pattard, 1990
Crustacea															
Daphnia magna	<24 h, IRCHA	Y	R	-	am	8.0±0.2	25±1	250	21 d	NOEC	reproduction and app. first offspring	0.27	3	6,7	Kühn et al., 1989
Daphnia magna	<24 h, IRCHA	Y	R	-	am	8.0±0.2	25±1	250	21 d	NOEC	reproduction and app. first offspring	0.14	2	6,5	Kühn et al., 1989

1 toxicity threshold is used as a NOEC

2 NOEC reported as TGK

3 light intensity 2800 lm; pH not adjusted

4 $1.5*10^4$ $cells.mL^{-1}$

5 value based on measured concentrations

6 photoperiod 9:15 light:dark with fluorescent light

7 nominal concentration; analysed concentration < 80% of the nominal concentration; renewal three times a week

8 value is the average of the two values reported for Kuhn *et al*. (1989)

9 TGK = Toxische Grenzkonzentration; defined as concentration where 3-5% inhibition occurs

10 dilution ranges not prepared properly

Table A1.8. Chronic toxicity of *m*-chlorotoluene to freshwater organisms.

For *m*-chlorotoluene no chronic freshwater data is available.

Table A1.9. Chronic toxicity of *p*-chlorotoluene to freshwater organisms.

Species	Species properties	Analysed	Test type	Substance purity	Test water	pH	Temp. [°C]	Hardness $CaCO_3$ [$mg.L^{-1}$]	Exp time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Ri	Notes	Reference
Crustacea															
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	EC50	reproduction	0.58	2	1,3	Hermens et al., 1984
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	NOEC	reproduction	0.32	2	1,3	Hermens et al., 1984
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	LC50	mortality	1.6	2	1,3	Hermens et al., 1984
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	NOEC	mortality	1	2	1,3	Hermens et al., 1984
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	EC50	growth	1.7	2	1,3	Hermens et al., 1985
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	NOEC	growth	0.32	2	1,3	Hermens et al., 1985
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	EC50	reproduction	1.3	2	1,3	De Wolf et al., 1988
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	NOEC	reproduction	0.56	2	1,3	De Wolf et al., 1988
Daphnia magna	< 24 h	Y	R		am		19±1		16 d	NOEC	growth	0.32	2	1,3	De Wolf et al., 1988
Pisces															
Danio rerio	24 h old eggs	Y	R	99	rw	7.4-8.4		210	28 d	NOEC	growth+hatch	1.9	2	2	Van Leeuwen et al., 1990

1 DSW used

2 renewal 3 times a week; concentrations were measured just before and after renewal, results given as mean measured concentration (60% of nominal)

3 value based on nominal concentration, measured concentration between 80% and 110% of nominal

Appendix 2. Detailed terrestrial toxicity data

Table A2.1. Toxicity of *o*-chlorotoluene to terrestrial organisms.

Species	Species properties	Soil type	Analysed	Substance purity	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [$mg.kg_{dw}^{-1}$]	Result std. Soil [$mg.kg_{dw}^{-1}$]	Ri	Notes	Reference
Macrophyta																
Avena sativa			N						14 d	EC50	biomass	89		4	1,2	OECD-SIDS 2000
Brassica rapa			N						14 d	EC50	biomass	>1000		4	1,2	OECD-SIDS 2000

1 result based on nominal concentration
2 no concentration of o.m. in the test soil given, therefore no result in standard soil calculated

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