National Institute
for Public Health
and the Environment

Report 601714005/2009

C.T.A. Moermond | E.H.W. Heugens

Environmental risk limits for trichlorophenols

rivm

RIVM Report 601714005/2009

Environmental risk limits for trichlorophenols

C.T.A. Moermond
E.H.W. Heugens

Contact:
Caroline Moermond
Expertise Centre for Substances
caroline.moermond@rivm.nl

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

RIVM, P.O. Box 1, 3720 BA Bilthoven, the Netherlands Tel +31 30 274 91 11 www.rivm.nl

rivm

Abstract

Environmental Risk Limits for trichlorophenols

The National Institute for Public Health and the Environment (RIVM) has derived environmental risk limits (ERLs) for six trichlorophenols in fresh and marine surface waters. The ERLs represent environmental concentrations of a substance offering different levels of protection to man and ecosystems. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the final environmental quality standard.

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 ecosystems specifically for short-term exposure (MAC_{eco}), and a concentration at which possible serious effects are to be expected (serious risk concentration, SRC_{eco}). Based on a preliminary screening of monitoring data, there is no indication that any of the newly derived ERLs is exceeded.

RIVM used the methodology as required by the European Water Framework Directive for derivation and selection of the ERLs. Potential risks for humans as well as effects on the aquatic ecosystem are taken into account.

The environmental quality standards are to be set by the Steering Committee for Substances. The ERLs as presented in this report are thus preliminary values that do not have an official status.

This report is part of a series. ERLs for 2,4-dichlorophenol and a series of monochlorophenols are reported separately.

Key words:
environmental risk limits, maximum permissible concentration, maximum acceptable concentration, trichlorophenols

rivm

Rapport in het kort

Milieurisicogrenzen voor trichloorfenolen

Het RIVM heeft milieurisicogrenzen voor zoet en zout oppervlaktewater afgeleid voor trichloorfenolen. Deze dienen als advieswaarden voor de Nederlandse Interdepartementale Stuurgroep Stoffen. De stuurgroep stelt de uiteindelijke milieukwaliteitsnormen vast.

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 vier milieurisicogrenzen: een niveau waarbij het risico verwaarloosbaar wordt geacht (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (maximaal toelaatbaar risiconiveau, MTR), de maximaal aanvaardbare concentratie voor ecosystemen, specifiek voor kortdurende blootstelling (MAC_{eco}) en een niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}). De nu afgeleide milieurisicogrenzen lijken op basis van een eerste vergelijking met monitoringsgegevens niet te worden overschreden.

Het RIVM heeft de afleiding en selectie van de milieurisicogrenzen uitgevoerd volgens de methodiek die is voorgeschreven door de Europese Kaderrichtlijn Water. Hierbij is zowel rekening gehouden met mogelijke risico's voor de mens als met eventuele effecten op het ecosysteem.

Omdat de uiteindelijke milieukwaliteitsnormen worden vastgesteld door de Nederlandse Interdepartementale Stuurgroep Stoffen, zijn de milieurisicogrenzen zoals afgeleid in dit rapport voorlopige waarden zonder officiële status.

Dit rapport is onderdeel van een serie. De milieurisicogrenzen voor 2,4-dichloorfenol en monochloorfenolen, 4-chloor-3-methylfenol en aminochloorfenol zijn in afzonderlijke rapporten opgenomen.

Trefwoorden:
milieurisicogrenzen, maximaal toelaatbaar risiconiveau, maximaal aanvaardbare concentratie, trichloorfenolen

rivm

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) that is incorporated in 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).

rivm

Acknowledgements

Thanks are due to J.M.C. Appelman, M.Sc., who is contact person at the Ministry of Housing, Spatial Planning and the Environment (VROM-DP) and to Dr. M.P.M. Janssen who is program coordinator for the derivation of ERLs within the RIVM.

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.

rivm

Contents

Summary

Environmental risk limits are derived using ecotoxicological, physico-chemical, 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 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 trichlorophenols in water. No risk limits were derived for the sediment compartment because sorption was assumed to be negligible.

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 (European Commission, 2003), and is incorporated in the guidance for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (Van Vlaardingen and Verbruggen, 2007). An overview of the derived ERLs is given in Table 1.

It should be noted that due to the mode of action of the trichlorophenols (narcosis), and the fact that these compounds often occur together, the use of the toxic unit approach is recommended. The toxic unit approach assumes that compounds that act similar, have concentration additive toxicity. This means that the sum of the ratio between measured concentration and risk limits for all trichlorophenols should not exceed 1.

Table 1. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values for trichlorophenols (in µg/L).

	MPC	MAC_{eco}	NC	SRC_{eco}
2,3,4-trichlorophenol				
Freshwater	0.54	12	5.4×10^{-3}	2.6×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	0.12	1.2	1.2×10^{-3}	2.6×10^{2}
2,3,5-trichlorophenol				
Freshwater	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
2,3,6-trichlorophenol				
Freshwater	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
2,4,5-trichlorophenol				
Freshwater	0.13	2.6	1.3×10^{-3}	1.9×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	0.13	2.0	1.3×10^{-3}	1.9×10^{2}
2,4,6-trichlorophenol				
Freshwater	0.26	32	2.6×10^{-3}	3.7×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine wate	0.26	3.2	2.6×10^{-3}	3.7×10^{2}
3,4,5-trichlorophenol				
Freshwater	0.20	2.0	2.0×10^{-3}	76
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	2.0×10^{-2}	0.20	2.0×10^{-4}	76

[a] n.a. = not applicable.
[b] n.d. = not derived due to a lack of data.

1 Introduction

1.1 Project framework

In this report, environmental risk limits (ERLs) for surface water (freshwater and marine) are derived for trichlorophenols for the project 'Standard setting for other relevant substances within the 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:

- 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 10^{-6} per year of death can be calculated (for carcinogenic substances). Within the scope of the Water Framework Directive, a probability of 10^{-6} on a life-time basis is used.

  Within the scope of the Water Framework Directive the MPC is specifically referring to long-term exposure.
- 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.

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 Environmental Risk Limits (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

ERLs are derived for trichlorophenols (Table 2), which are selected by the Netherlands in the scope of the Water Framework Directive (WFD; 2000/60/EC). The derivation of environmental risk limits for monochlorophenols, dichlorophenols, aminochlorophenol and 4-chloro-3-methylphenol will be reported in separate reports (Moermond and Heugens, 2009ab).

Table 2. Selected compounds.

Compound	CAS number
2,3,4-trichlorophenol	15950-66-0
2,3,5-trichlorophenol	933-78-8
2,3,6-trichlorophenol	933-75-5
2,4,5-trichlorophenol	95-95-4
2,4,6-trichlorophenol	88-06-2
3,4,5-trichlorophenol	609-19-8

1.2.1 Use and mode of action

The main use of chlorophenols in general, is as an intermediate for manufacturing pesticides, biocides, dyes and pharmaceuticals (Muller, 2008). Individual chlorophenols have been used as mothproofing agents, miticides, germicides, algicides, fungicides, biocides, and wood preservatives (National Pollutant Inventory, 2005). 2,4,6-Trichlorophenol was previously used as an antiseptic, a pesticide for wood, leather, and glue preservation and as an anti-mildew treatment (National Pollutant Inventory, 2005).

The mode of action of chlorophenols is mainly narcosis. Furthermore, chlorophenols can uncouple the oxidative phosphorylation and inhibit the electron transport system in algae and plants.

2 Methods

2.1 General

The methodology for the data selection and derivation of ERLs is described in detail in 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) and prepared within the context of the WFD.

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

In accordance with the WFD, data of existing evaluations were used as a starting point. 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 potentially relevant references in the RIVM e-tox base and EPA's ECOTOX database were checked.

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 (see section 2.2.2 and 2.3.2).

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 Derivation of ERLs

2.3.1 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_{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}.

2.3.2 $MAC_{eco, marine}$

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

2.3.3 Toxic unit approach

Due to the mode of action of the trichlorophenols (narcosis), and the fact that these compounds often occur together, the use of the toxic unit approach is recommended. The toxic unit approach assumes that compounds that act similar, have concentration additive toxicity. This means that the sum of the ratio between measured concentration and risk limits for all trichlorophenols should not exceed 1.

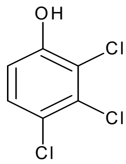
3 Derivation of environmental risk limits

3.1 2,3,4-trichlorophenol

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

3.1.1.1 Identity

Table 3. Identification of 2,3,4-trichlorophenol.

Chemical name	2,3,4-trichlorophenol
CAS number	15950-66-0
EC number	240-083-2
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc1ccc(Cl)c(Cl)c1Cl

3.1.1.2 Physico-chemical properties

Table 4. Physico-chemical properties of 2,3,4-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**500**	Recommended by reference	Mackay et al., 2000
		97.5	EpiWin	US EPA, 2007
pK_a	[-]	7.66	Recommended by reference	Mackay et al., 2000
		6.97	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	**3.80**	Recommended by reference	Mackay et al., 2000
		3.45	EpiWin	US EPA, 2007
		3.48	Calculated (ClogP)	BioByte, 2006
log K_{OC}	[-]	3.08	EpiWin	US EPA, 2007
		3.29	Calculated using log K_{OW} = 3.80 (QSAR for phenols)	According to Sabljic et al., 1995
Vapour pressure	[Pa]	1.00	25 ºC, solid	Mackay et al., 2000
		3.48	25 ºC, liquid	Mackay et al., 2000
		0.328	EpiWin	US EPA, 2007
Melting point	[°C]	83.5		Muller, 2008
		79-81	Recommended by reference	Mackay et al., 2000
		63.8	EpiWin	US EPA, 2007
Boiling point	[°C]	-	Sublimates	Muller, 2008
Henry's law constant	[Pa.m^3/mol]	0.66	EpiWin	US EPA, 2007

3.1.1.3 Behaviour in the environment

Table 5. Selected environmental properties of 2,3,4-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]	Unknown		
Photolysis half-life	DT50 [h]	1.7	Xenotest 200	Mackay et al., 2000
Readily biodegradable		Unknown		
Degradability	DT50	Unknown		
Relevant metabolites		Unknown		

Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.1.1.4 Bioconcentration and biomagnification

Bioaccumulation data for 2,3,4-trichlorophenol are tabulated in Table 6. No experimental bioaccumulation data were available.

Table 6. Overview of bioaccumulation data for 2,3,4-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	339	Calculated using log K_{OW} = 3.80	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} < 4.5.	

3.1.1.5 Human toxicological treshold limits and carcinogenicity

2,3,4-trichlorophenol does not have an R-classification. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 $\mu g/kg_{bw}$/day (U.S. EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.1.2 Trigger values

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

Table 7. 2,3,4-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp-water}$	2.29	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.1.1.2
BCF	339	[L/kg]		3.1.1.4
BMF	1	[kg/kg]		3.1.1.4
Log K_{OW}	3.80	[-]		3.1.1.2
R-phrases	No R-phrases	[-]		3.1.1.5
A1 value	1	[µg/L]	Mandatory for phenols	
DW standard	-	[µg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 2,3,4-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2,3,4-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 2,3,4-trichlorophenol has a log $K_{OW} \geq 3$; assessment of secondary poisoning is triggered.
- 2,3,4-trichlorophenol does not have any R-classifications, but is classified as a possible carcinogenic. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) has to be derived.
- For 2,3,4-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 μg/L for phenols applies.

3.1.3 Aquatic toxicity data

3.1.3.1 Toxicity data

An overview of the selected toxicity data for 2,3,4-trichlorophenol is given in Table 8 for freshwater and in Table 9 for the marine environment. Detailed toxicity data for 2,3,4-trichlorophenol are tabulated in Appendix 2.

Table 8. 2,3,4-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	13
		Bacteria	1.9
		Bacteria	3.0
		Algae	2.0
		Crustacea	2.2
		Pisces	1.9
		Pisces	**1.2**
		Pisces	2.6

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.

Table 9. 2,3,4-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute** [a] **Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	2.8[b]

[a] For detailed information see Appendix 2.
[b] Geometric mean of 1.25, 4.13, and 4.44 mg/L; endpoint bioluminescence for *Vibrio fischeri*.

3.1.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 2,3,4-trichlorophenol are combined.

3.1.4 Derivation of Environmental Risk Limits

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

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

Acute toxicity data are available for bacteria, algae, crustacea (*Daphnia*) and fish: the base set is complete. No chronic data are available. Lepper (2005) states that no MPC can be derived on the basis of acute toxicity data alone. However, since data are available for the (chronic) 'human exposure through the consumpion of fishery products' route, and since chronic data are available for other trichlorophenols which show a similar toxicity ('read-across'), it is decided to derive an MPC_{eco} on the basis of acute toxicity.

The lowest LC50 is 1.2 mg/L the fish *Leuciscus idus melanotus*. This value is higher than the 44-hours LOEC for *Hydra* of 1 mg/L (See Table A2.2 in Appendix 2). With an assessment factor of 1000, the $MPC_{eco, water}$ becomes 1.2 / 1000 = 1.2×10^{-3} mg/L = 1.2 µg/L. For the marine environment, with an assessment factor of 10000, the $MPC_{eco, marine}$ becomes 1.2 / 10000 = 1.2×10^{-4} mg/L = 0.12 µg/L.

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

2,3,4-trichlorophenol has a log $K_{OW} \geq 3$, thus assessment of secondary poisoning is triggered. No bird or mammal data for 2,3,4-trichlorophenol are available. Regarding the other trichlorophenols, only bird and mammal data are available for 2,4,6-trichlorophenol. Thus, to obtain an *indication* on the relevance of the exposure route, the lowest MPC_{oral} (3.3 mg/kg) for 2,4,6-trichlorophenol is used (see section 3.5.4.1). Subsequently, the $MPC_{sp, water}$ can be calculated using a BCF of 339 L/kg and a BMF of 1 kg/kg (section 3.1.1.4) and becomes 3.3 / (339 × 1) = 9.7×10^{-3} mg/L = 9.7 µg/L.

For the marine environment, an extra biomagnification factor should be used. But since this factor is also 1 by default for compounds with log K_{OW} < 4.5, the $MPC_{sp, marine}$ equals the $MPC_{sp, water}$ and is also 9.7 µg/L.

$MPC_{hh\ food, water}$

Derivation of $MPC_{hh\ food, water}$ for 2,3,4-trichlorophenol is triggered (Table 7). With an ADI of 0.003 $mg/kg_{bw}/d$ for chlorophenols, a BCF of 339 L/kg and a BMF of 1 kg/kg (section 3.1.1.4) , the $MPC_{hh\ food}$ becomes (0.1 × 0.003 × 70) / 0.115 = 0.183 mg/L. Subsequently, the $MPC_{hh\ food, water}$ and $MPC_{hh\ food, marine}$ become 0.183/ (339 × 1) = 0.00054 mg/L = 0.54 µg/L.

$MPC_{dw, water}$

The $MPC_{dw, water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC.

For the freshwater environment, the lowest MPC is the value for human consumption of fishery products (0.54 µg/L). Thus, the overall MPC_{water} is 0.54 µg/L.

For the marine environment, the lowest MPC is the value for direct toxicity to aquatic ecosystems (0.12 µg/L). Thus, the overall MPC_{marine} is 0.12 µg/L.

3.1.4.2 Derivation of MAC_{eco}

The base set for acute data is complete. 2,3,4-chlorophenol has a BCF > 100 L/kg, a non-specific mode of action (polar narcosis) and the interspecies variation is low. Thus, an assessment factor of 100 can be applied on the lowest LC50, and the $MAC_{eco,\ water}$ becomes 1.2 / 100 = 1.2×10^{-2} mg/L = 12 µg/L.

For the $MAC_{eco,\ marine}$ an additional assessment factor of 10 should be applied since no specific marine taxa are present in the dataset. Thus, the $MAC_{eco,\ marine}$ becomes
1.2 / 1000 = 1.2×10^{-3} mg/L = 1.2 µg/L.

3.1.4.3 Derivation of NC

The NC is derived by dividing the final MPC by a factor of 100.

$NC_{water} = 5.4 \times 10^{-3}$ µg/L.
$NC_{marine} = 1.2 \times 10^{-3}$ µg/L.

3.1.4.4 Derivation of SRC_{eco}

The $SRC_{eco,\ water}$ and $SRC_{eco,\ marine}$ can be derived using the geometric mean of all acute freshwater and marine L(E)C50 data (2.6 mg/L) with an assessment factor of 10. These data are not normally distributed (only significant at the 0.01 level using the Anderson-Darling test for normality). The $SRC_{eco,\ water}$ and $SRC_{eco,\ marine}$ are set at 2.6 / 10 = 0.26 mg/L = 260 µg/L.

3.1.5 Sediment compartment

The log $K_{p,\ susp\text{-}water}$ of 2,3,4-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.1.6 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 10.

Table 10. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values for 2,3,4-trichlorophenol (in µg/L).

ERL	Unit	MPC	MAC_{eco}	NC	SRC_{eco}
Freshwater	µg/L	0.54	12	5.4×10^{-3}	2.6×10^{2}
Drinking water	µg/L	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	µg/L	0.12	1.2	1.2×10^{-3}	2.6×10^{2}

[a] n.a. = not applicable.

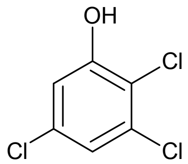
Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of 2,3,4-trichlorophenol in water was below detection limits (0.02 µg/L).

3.2 2,3,5-trichlorophenol

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

3.2.1.1 Identity

Table 11. Identification of 2,3,5-trichlorophenol.

Chemical name	2,3,5-trichlorophenol
CAS number	933-78-8
EC number	213-272-2
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc1cc(Cl)cc(Cl)c1Cl

3.2.1.2 Physico-chemical properties

Table 12. Physico-chemical properties of 2,3,5-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**500**	25 ºC;	Mackay et al., 2000
		144	EpiWin	US EPA, 2007
pK_a	[-]	7.37	Recommended by reference	Mackay et al., 2000
		6.43	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	**3.69**	Recommended by reference	Mackay et al., 2000
		3.60	Calculated (ClogP)	BioByte, 2006
		3.45	EpiWin	US EPA, 2007
log K_{OC}	[-]	**3.22**	Calculated using log K_{OW}=3.69 QSAR for phenols)	According to Sabljic et al., 1995
		3.07	EpiWin	US EPA, 2007
Vapour pressure	[Pa]	1	25 ºC, solid	Mackay et al., 2000
		2.32	25 ºC, solid	Mackay et al, 2000
		0.328	EpiWin	US EPA, 2007
Melting point	[°C]	62		Mackay et al, 2000
		63.8	EpiWin	US EPA, 2007
		62		Muller, 2008
Boiling point	[°C]	262	EpiWin	US EPA, 2007
		248-249		Muller, 2008
Henry's law constant	[Pa.m^3/mol]	0.39	Calculated by Mackay	Mackay et al., 2000
		0.45	EpiWin	US EPA, 2007

3.2.1.3 Behaviour in the environment

No specific information on environmental behaviour of 2,3,5-trichlorophenol is available. Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.2.1.4 Bioconcentration and biomagnification

Bioaccumulation data for 2,3,5-trichlorophenol are tabulated in Table 13. No experimental bioaccumulation data are available.

Table 13. Overview of bioaccumulation data for 2,3,5-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	273	Calculated using log K_{OW} = 3.69	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} <4.5	

3.2.1.5 Human toxicological treshold limits and carcinogenicity

2,3,5-trichlorophenol does not have an R-classification. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 μg/kg_{bw}/day (U.S. EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.2.2 Trigger values

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

Table 14. 2,3,5-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp-water}$	2.22	[-]	$K_{OC} \times f_{OC,susp}$[1]	K_{OC}: 3.2.1.2
BCF	273	[L/kg]		3.2.1.4
BMF	1	[kg/kg]		3.2.1.4
Log K_{OW}	3.69	[-]		3.2.1.2
R-phrases	No R-phrases	[-]		3.2.1.5
A1 value	1	[μg/L]	Mandatory for phenols	
DW standard	-	[μg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 2,3,5-trichlorophenol has a log $K_{p,\ susp-water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2,3,5-trichlorophenol has a log $K_{p,\ susp-water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 2,3,5-trichlorophenol has a log $K_{OW} \geq$ 3; assessment of secondary poisoning is triggered.
- 2,3,5-trichlorophenol does not have any R-classifications, but is classified as a possible carcinogenic. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) has to be derived.
- For 2,3,5-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 μg/L for phenols applies.

3.2.3 Aquatic toxicity data

3.2.3.1 Toxicity data

An overview of the selected toxicity data for 2,3,5-trichlorophenol is given in Table 15 for freshwater and in Table 16 for the marine environment. Detailed toxicity data for 2,3,5-trichlorophenol are tabulated in Appendix 2.

Table 15. 2,3,5-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a]		**Acute**[a]	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	1.3
		Bacteria	4.9
		Protozoa	0.84
		Crustacea	2.3
		Pisces	1.4
		Pisces	**0.62**
		Pisces	0.88[b]
		Pisces	0.8
		Pisces	1.3

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.
[b] most senstive pH (6.1), parameter mortality for *Poecilia reticulata.*

Table 16. 2,3,5-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a]		**Acute** [a]	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	0.86[b]

[a] For detailed information see Appendix 2.
[b] geomean of 1.11 and 0.67 mg/L, parameter bioluminescence for *Vibrio fischeri.*

3.2.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 2,3,5-trichlorophenol are combined.

3.2.4 Derivation of Environmental Risk Limits

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

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

Acute toxicity data are available for bacteria, protozoa, crustacea (*Daphnia*) and pisces, not for algae. Thus, the base set is not complete. No chronic data are available. Because no algal data are present, and read across is not possible because algae have been shown to be sensitive to this group of compounds and may thus be the most sensitive of all species, no $MPC_{eco,\ water}$ can be derived using assessment factors.

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

2,3,5-trichlorophenol has a log $K_{OW} \geq 3$, thus assessment of secondary poisoning is triggered. No bird or mammal data for 2,3,5-trichlorophenol are available. Regarding the other trichlorophenols, only bird and mammal data are available for 2,4,6-trichlorophenol. Thus, to obtain an *indication* on the relevance of the exposure route, the lowest MPC_{oral} (3.3 mg/kg) for 2,4,6-trichlorophenol is used (see section 3.5.4.1). Subsequently, the $MPC_{sp, water}$ can be calculated using a BCF of 273 L/kg and a BMF of 1 kg/kg (section 3.2.1.4) and becomes 3.3 / (273 × 1) = 1.2×10^{-2} mg/L = 12 µg/L.

For the marine environment, an extra biomagnification factor should be used. But since this factor is 1 by default for compounds with log K_{OW} < 4.5, the $MPC_{sp, marine}$ equals the $MPC_{sp, water}$ and is also 12 µg/L.

$MPC_{hh food, water}$

Derivation of $MPC_{hh food, water}$ for 2,3,5-trichlorophenol is triggered (Table 14). With an ADI of 0.003 $mg/kg_{bw}/d$ for chlorophenols, a BCF of 273 L/kg and a BMF of 1 kg/kg (section 3.2.1.4), the $MPC_{hh food}$ becomes (0.1 × 0.003 × 70) / 0.115 = 0.183 mg/L. Subsequently, the $MPC_{hh food, water}$ and $MPC_{hh food, marine}$ become 0.183 / (273 × 1) = 0.00067 mg/L = 0.67 µg/L.

$MPC_{dw, water}$

The $MPC_{dw, water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC. However, no $MPC_{eco, water}$ and $MPC_{eco, marine}$ could be derived due to the absence of algal toxicity data. Thus, no final MPC_{water} and MPC_{marine} can be selected for 2,3,5-trichlorophenol.

3.2.4.2 Derivation of MAC_{eco}

The base set is not complete, so no MAC_{eco} can be derived for 2,3,5-trichlorophenol.

3.2.4.3 Derivation of NC

No MPC has been derived, so no NC can be derived for 2,3,5-trichlorophenol.

3.2.4.4 Derivation of SRC_{eco}

The base set is not complete, so no SRC_{eco} can be derived for 2,3,5-trichlorophenol.

3.2.5 Sediment compartment

The log $K_{p, susp-water}$ of 2,3,5-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.2.6 Comparison of derived ERLs with monitoring data

ERLs for 2,3,5-trichlorophenol could not be derived.

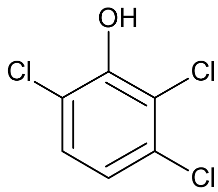
Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of 2,3,5-trichlorophenol in water was below detection limits (0.02 µg/L).

3.3 2,3,6-trichlorophenol

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

3.3.1.1 Identity

Table 17. Identification of 2,3,6-trichlorophenol.

Chemical name	2,3,6-trichlorophenol
CAS number	933-75-5
EC number	213-271-7
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc(c(ccc1Cl)Cl)c1Cl

3.3.1.2 Physico-chemical properties

Table 18. Physico-chemical properties of 2,3,6-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**450**		Mackay et al., 2000
		190	EpiWin	US EPA, 2007
pK_a	[-]	7.13	Recommended by reference	Mackay et al., 2000
		6.03	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	**3.46**	MlogP; recommended by reference)	BioByte, 2006
		3.27	ClogP (calculated)	BioByte, 2006
		3.8	Recommended by reference	Mackay et al., 2000
		3.45	EpiWin	US EPA, 2007
log K_{OC}	[-]	**3.08**	Calculated using log K_{OW} = 3.46 (QSAR for phenols)	According to Sabljic et al., 1995
		3.08	EpiWin	US EPA, 2007
Vapour pressure	[Pa]	0.328	EpiWin	US EPA, 2007
Melting point	[°C]	58	Recommended by reference	Mackay et al., 2000
		63.8	EpiWin	US EPA, 2007
		101		Muller, 2008
Boiling point	[°C]	262	EpiWin	US EPA, 2007
		272		Muller, 2008
Henry's law constant	[Pa.m^3/mol]	0.340	EpiWin	US EPA, 2007

3.3.1.3 Behaviour in the environment

No specific information on environmental behaviour is available for 2,3,6-trichlorophenol. Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.3.1.4 Bioconcentration and biomagnification

Bioaccumulation data for 2,3,6-trichlorophenol are tabulated in Table 19. No experimental bioaccumulation data were available.

Table 19. Overview of bioaccumulation data for 2,3,6-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	174	Calculated using log K_{OW} = 3.46	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} < 4.5.	

3.3.1.5 Human toxicological treshold limits and carcinogenicity

2,3,6-trichlorophenol has the following R-phrases: R20/21/22; R36/37/38. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 μg/kg_{bw}/day (US EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.3.2 Trigger values

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

Table 20. 2,3,6-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	2.08	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.3.1.2
BCF	174	[L/kg]		3.3.1.4
BMF	1	[kg/kg]		3.3.1.4
Log K_{OW}	3.46	[-]		3.3.1.2
R-phrases	R20/21/22; R36/37/38	[-]		3.3.1.5
A1 value	1	[μg/L]	Mandatory for phenols	
DW standard	-	[μg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 2,3,6-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2,3,6-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 2,3,6-trichlorophenol has a log $K_{OW} \geq$ 3; assessment of secondary poisoning is triggered.
- 2,3,6-trichlorophenol has a R21/22 classification, a BCF > 100 L/kg, and is classified as a possible carcinogenic. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) has to be derived.
- For 2,3,6-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 μg/L for phenols applies.

3.3.3 Aquatic toxicity data

3.3.3.1 Toxicity data

An overview of the selected toxicity data for 2,3,6-trichlorophenol is given in Table 21 for freshwater and in Table 22 for the marine environment. Detailed toxicity data for 2,3,6-trichlorophenol are tabulated in Appendix 2.

Table 21. 2,3,6-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	5.7
		Bacteria	18
		Crustacea	5.4[b]
		Crustacea	7.4
		Pisces	7.4
		Pisces	1.9
		Pisces	2.9
		Pisces	0.95

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.
[b] most sensitive pH (6.5), parameter mortality for *Astacus fluviatilis.*
[c] most senstive pH (6.1), parameter mortality for *Poecilia reticulata.*

Table 22. 2,3,6-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute** [a] **Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	5.2[b]

[a] For detailed information see Appendix 2.
[b] geometric mean of 12.7 and 2.1 mg/L; parameter bioluminescence for *Vibrio fischeri.*

3.3.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 2,3,6-trichlorophenol are combined.

3.3.4 Derivation of Environmental Risk Limits

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

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

Acute toxicity data are available for bacteria, protozoa, crustacea (*Daphnia*) and pisces, not for algae. Thus, the base set is not complete. No chronic data are available. Because no algal data are present, and read across is not possible because algae have been shown to be sensitive to this group of compounds and may thus be the most sensitive of all species, no $MPC_{eco, water}$ can be derived using assessment factors.

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

2,3,6-trichlorophenol has a log $K_{OW} \geq 3$, thus assessment of secondary poisoning is triggered. No bird or mammal data for 2,3,6-trichlorophenol are available. Regarding the other trichlorophenols, only bird and mammal data are available for 2,4,6-trichlorophenol. Thus, to obtain an *indication* on the relevance of the exposure route, the lowest MPC_{oral} (3.3 mg/kg) for 2,4,6-trichlorophenol is used (see section 3.5.4.1). Subsequently, the $MPC_{sp, water}$ can be calculated using a BCF of 176 L/kg and a BMF of 1 kg/kg (section 3.3.1.4) and becomes 3.3 / (176 × 1) = 1.9×10^{-2} mg/L = 19 µg/L.

For the marine environment, an extra biomagnification factor should be used. But since this factor is 1 by default for compounds with log $K_{OW} < 4.5$, the $MPC_{sp, marine}$ equals the $MPC_{sp, water}$ and is also 19 µg/L.

$MPC_{hh food, water}$

Derivation of $MPC_{hh food, water}$ for 2,3,6-trichlorophenol is triggered (Table 20). With an ADI of 0.003 $mg/kg_{bw}/d$ for phenols, a BCF of 174 L/kg and a BMF of 1 kg/kg (section 3.3.1.4) , the $MPC_{hh food}$ becomes (0.1 × 0.003 × 70) / 0.115 = 0.183 mg/L. Subsequently, the $MPC_{hh food, water}$ and $MPC_{hh food, marine}$ become 0.183 / (174 × 1) = 0.00104 mg/L = 1.04 µg/L.

$MPC_{dw, water}$

The $MPC_{dw, water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC. However, no $MPC_{eco, water}$ and $MPC_{eco, marine}$ could be derived due to the absence of algal toxicity data. Thus, no final MPC_{water} and MPC_{marine} can be selected for 2,3,6-trichlorophenol.

3.3.4.2 Derivation of MAC_{eco}

The base set is not complete, so no MAC_{eco} can be derived for 2,3,6-trichlorophenol.

3.3.4.3 Derivation of NC

No MPC has been derived, so no NC can be derived for 2,3,6-trichlorophenol.

3.3.4.4 Derivation of SRC_{eco}

The base set is not complete, so no SRC_{eco} can be derived for 2,3,6-trichlorophenol.

3.3.5 Sediment compartment

The log $K_{p, susp\text{-}water}$ of 2,3,6-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.3.6 Comparison of derived ERLs with monitoring data

ERLs for 2,3,6-trichlorophenol could not be derived.

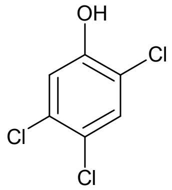
Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of 2,3,6-trichlorophenol in water was below detection limits (0.02 µg/L).

3.4 2,4,5-trichlorophenol

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

3.4.1.1 Identity

Table 23. Identification of 2,4,5-trichlorophenol.

Chemical name	2,4,5-trichlorophenol
Product/Trade names	Collunosol Dowicide 2 Preventol i
CAS number	95-95-4
EC number	202-467-8
Annex I Index number	604-017-00-X
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc(c(cc(c1Cl)Cl)Cl)c1

3.4.1.2 Physico-chemical properties

Table 24. Physico-chemical properties of 2,4,5-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**948**	25 ºC; pH 5.1; recommended by reference	Mackay et al., 2000
		114	EpiWin	US EPA, 2007
pK_a	[-]	7.43	Recommended by reference	Mackay et al., 2000
		6.70	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	**3.72**	Recommended by reference	Mackay et al., 2000
		3.72	MlogP; recommended by reference)	BioByte, 2006
		3.60	ClogP (calculated)	BioByte, 2006
		3.45	EpiWin	US EPA, 2007
log K_{OC}	[-]	**3.14**	Geomean, values from soil, lake, river sediment	Howard, 1991; cited in Mackay et al., 2000
		3.24	Calculated using log K_{OW} = 3.72 (QSAR for phenols)	According to Sabljic et al., 1995
		3.07	EpiWin	US EPA, 2007

Parameter	Unit	Value	Remark	Reference
Vapour pressure	[Pa]	2.5	25 ºC, solid, recommended by reference	Mackay et al., 2000
		6.76	25 ºC, liquid, recommended by reference	Mackay et al., 2000
		0.328	EpiWin	US EPA, 2007
Melting point	[°C]	68-70	Recommended by reference	Mackay et al., 2000
		63.8	EpiWin	US EPA, 2007
		68		Muller, 2008
Boiling point	[°C]	244-250	Recommended by reference	Mackay et al., 2000
		262	EpiWin	US EPA, 2007
		245-246		Muller, 2008
Henry's law constant	[Pa.m^3/mol]	0.52	Recommended by reference EpiWin	Mackay et al., 2000
		0.57		US EPA, 2007

3.4.1.3 Behaviour in the environment

Table 25. Selected environmental properties of 2,4,5-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [yr]	>8 × 10^6		Howard, 1991 in Mackay et al., 2000
Photolysis half-life	DT50 [hr]	0.5-1.0	Natural and estuarine water, sunlight	Howard, 1991 in Mackay et al., 2000
Readily biodegradable		Unknown		
Degradability	DT50 [d]	690	river water	Howard, 1991 in Mackay et al., 2000
Relevant metabolites		Unknown		

Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.4.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for 2,4,5-trichlorophenol is given in Table 26. Detailed bioaccumulation data for 2,4,5-trichlorophenol are tabulated in Appendix 1.

Table 26. Overview of bioaccumulation data for 2,4,5-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	1414		Call et al., 1980
BMF	[kg/kg]	1	Default value for compounds with BCF < 2000 L/kg.	

3.4.1.5 Human toxicological treshold limits and carcinogenicity

2,4,5-trichlorophenol has the following R-phrases relating to human toxicology: R22, R36/38. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 μg/kg$_{bw}$/day (U.S. EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.4.2 Trigger values

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

Table 27. 2,4,5-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp-water}$	2.14	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.4.1.2
BCF	1414	[L/kg]		3.4.1.4
BMF	1	[kg/kg]		3.4.1.4
Log K_{OW}	3.72	[-]		3.4.1.2
R-phrases	R22, R36/38, R50/53	[-]		3.4.1.5
A1 value	1	[µg/L]	Mandatory for phenols	
DW standard	-	[µg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 2,4,5-trichlorophenol has a log $K_{p, susp-water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2,4,5-trichlorophenol has a log $K_{p, susp-water}$ < 3; expression of the MPC_{water} as $MPC_{susp, water}$ is not required.
- 2,4,5-trichlorophenol has a BCF ≥ 100 L/kg; assessment of secondary poisoning is triggered.
- 2,4,5-trichlorophenol has a BCF ≥ 100 L/kg and an R22 classification, and is a possible carcinogenic. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.
- For 2,4,5-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 µg/L for phenols applies.

3.4.3 Aquatic toxicity data

3.4.3.1 Toxicity data

An overview of the selected toxicity data for 2,4,5-trichlorophenol is given in Table 28 for freshwater and in Table 29 for the marine environment. Detailed toxicity data for 2,4,5-trichlorophenol are tabulated in Appendix 2.

Table 28. 2,4,5-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a] Taxonomic group	NOEC/EC10 (mg/L)	Acute[a] Taxonomic group	L(E)C50 (mg/L)
Algae	**0.10**	Bacteria	12
Algae	0.24	Bacteria	1.2
Cyanobacteria	0.12	Bacteria	11
Crustacea	0.38[b]	Protozoa	1.57[d]
Pisces	0.11	Macrophyta	0.56[e]
Pisces	0.16[c]	Fungi	4.3
		Fungi	2.0
		Fungi	5.9
		Crustacea	1.45[f]
		Crustacea	0.29[g]
		Annelida	0.90
		Pisces	1.7
		Pisces	0.40[h]
		Pisces	0.45
		Pisces	0.63[i]
		Pisces	**0.26**
		Pisces	13
		Pisces	0.95[j]
		Pisces	0.99[k]
		Pisces	0.90
		Pisces	3.0

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.
[b] Most sensitive endpoint, parameter 'number of offspring' for *Ceriodaphnia dubia.*
[c] Most sensitive endpoint, parameter survival for *Pimephales promelas.*
[d] Most relevant endpoint, parameter growth rate for *Tetrahymena pyriformis.*
[e] Most sensitive pH (5.8), parameter yield (dry weight) for *Lemna minor.*
[f] Geometric mean of 1.74 and 1.21 mg/L, paramter mortality/immobility for *Ceriodaphnia dubia.*
[g] Most sensitive pH (6.2), parameter mortality for *Daphnia magna.*
[h] Most sensitive life stage, parameter mortality for *Danio rerio.*
[i] Geometric mean of 1.0 and 0.4 mg/L, parameter mortality for *Leuciscus idus melanotus.*
[j] Geometric mean of 0.90, 0.74, and 1.27 mg/L, parameter mortality for *Pimephales promelas.*
[k] Most sensitive pH (6.0), parameter mortality for *Poecilia reticulata.*

Table 29. 2,4,5-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a] Taxonomic group	NOEC/EC10 (mg/L)	Acute [a] Taxonomic group	L(E)C50 (mg/L)
Bacteria	0.44	Bacteria	0.60[c]
Algae	0.23[b]	Annelida	2.6[d]
		Crustacea	0.64[e]
		Crustacea	2.4
		Pisces	1.7

[a] For detailed information see Appendix 2.
[b] Most sensitive life stage, parameters vegetative growth and number of reproductive structures for *Champia parvula.*
[c] Most sensitive pH (6.2), parameter bioluminescence for *Vibrio fischeri.*
[d] Most sensitive life-stage, parameter embryo development for *Platynereis durnerilii.*
[e] Most sensitive life-stage, paramteter mortality for *Palaemonetes pugio.*

3.4.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 2,4,5-trichlorophenol are combined.

3.4.4 Derivation of Environmental Risk Limits

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

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

Acute toxicity data are available for bacteria, protozoa, macrophyta, fungi, annelida, crustacea, and fish. Chronic toxicity data are available for bacteria, algae, crustacea and fish. Although the acute dataset lacks algal toxicity data, it is assumed that the base set is complete due to the presence of acute macrophyte data (another primary producer), and the number of trophic levels present in the dataset.

Chronic data are available for algae, crustacea and fish. The taxon with the lowest acute LC50 (fish) is also present in the chronic dataset. For the derivation of the $MPC_{eco,\ water}$, an assessment factor of 10 can be used on the lowest NOEC (0.10 mg/L for the algae *Nitzschia* sp.). Thus, the $MPC_{eco,\ water}$ becomes 0.10 / 10 = 0.01 mg/L = 10 µg/L.

For the marine environment, an assessment factor of 50 can be used because data are available for the typically marine rhodophyte *Champia parvula*. Thus, the $MPC_{eco,\ marine}$ becomes 0.10 / 50 = 0.002 mg/L = 2 µg/L.

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

2,4,5-trichlorophenol has a BCF ≥ 100 L/kg, thus assessment of secondary poisoning is triggered. No bird or mammal data for 2,4,5-trichlorophenol are available. Regarding the other trichlorophenols, only bird and mammal data are available for 2,4,6-trichlorophenol. Thus, to obtain an *indication* on the relevance of the exposure route, the lowest MPC_{oral} (3.3 mg/kg) for 2,4,6-trichlorophenol is used (see section 3.5.4.1). Subsequently, the $MPC_{sp,\ water}$ can be calculated using a BCF of 1414 L/kg and a BMF of 1 kg/kg (section 3.4.1.4) and becomes $3.3 / (1414 \times 1) = 2.3 \times 10^{-3}$ mg/L = 2.3 µg/L.

For the marine environment, an extra biomagnification factor should be used. But since this factor is 1 by default for compounds with BCF < 2000 L/kg, the $MPC_{sp,\ marine}$ equals the $MPC_{sp,\ water}$ and is also 2.3 µg/L.

$MPC_{hh\ food,\ water}$

Derivation of $MPC_{hh\ food,\ water}$ for 2,4,5-trichlorophenol is triggered (Table 27). With an ADI of 0.003 $mg/kg_{bw}/d$ for phenols, a BCF of 1414 L/kg and a BMF of 1 kg/kg (section 3.4.1.4) , the $MPC_{hh\ food}$ becomes $(0.1 \times 0.003 \times 70) / 0.115 = 0.183$ mg/L. Subsequently, the $MPC_{hh\ food,\ water}$ and $MPC_{hh\ food,\ marine}$ become $0.183 / (1414 \times 1) = 0.00013$ mg/L = 0.13 µg/L.

$MPC_{dw,\ water}$

The $MPC_{dw,\ water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC.

For the freshwater environment, the lowest MPC value is the value for human consumption of fishery products of 0.13 μg/L. Thus, the overall MPC_{water} is 0.13 μg/L.

For the marine environment, the lowest MPC value is the value for human consumption of fishery products of 0.13 μg/L. Thus, the overall MPC_{marine} is 0.13 μg/L.

3.4.4.2 Derivation of MAC_{eco}

Assuming the base set is complete, the $MAC_{eco, water}$ can be derived using an assessment factor of 100. The compound has potential to bioaccumulate, the mode of action (narcosis) is non-specific and interspecies variation is low. The difference between the lowest acute LC50 (for fish) and the lowest chronic NOEC (for algae) is a factor of 2.6. Algae are not present in the acute dataset, but for algae, bioaccumulation is not important. For fish bioaccumulation may be important, and this is reflected in the assessment factor of 100 on the lowest LC50 of 0.26 mg/L for the fish *Oncorhynchus mykiss*. Thus, the $MAC_{eco, water}$ becomes 0.26 / 100 = 0.0026 mg/L = 2.6 μg/L.

The $MAC_{eco, marine}$ should be derived with an additional assessment factor of 5 (due to the presence of the typically marine rhodophyte *Champia parvula* in the dataset) and becomes 0.26 / 500 = 0.00052 mg/L = 0.52 μg/L. However, the $MAC_{eco, marine}$ can not be lower than the MPC_{marine} (2.0 μg/L). Thus, the $MAC_{eco, marine}$ is set equal to the MPC_{marine} and becomes 2.0 μg/L.

3.4.4.3 Derivation of NC

The NC is derived by dividing the final MPC by a factor of 100.

$NC_{water} = 1.3 \times 10^{-3}$ μg/L.
$NC_{marine} = 1.3 \times 10^{-3}$ μg/L.

3.4.4.4 Derivation of SRC_{eco}

The geometric mean of all chronic data is 0.19 mg/L. These data are normally distributed (significant at all levels using the Anderson-Darling test for normality). Because more than three NOECs are available, no comparison has to be made with the geometric mean of the acute data. Thus, the $SRC_{eco, water}$ and $SRC_{eco, marine}$ are set at 0.19 mg/L = 190 μg/L.

3.4.5 Sediment compartment

The log $K_{p, susp\text{-}water}$ of 2,4,5-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.4.6 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 30.

Table 30. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values for 2,4,5-trichlorophenol (in μg/L).

ERL	Unit	MPC	MAC_{eco}	NC	SRC_{eco}
Freshwater	μg/L	0.13	2.6	1.3×10^{-3}	1.9×10^{2}
Drinking water	μg/L	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	μg/L	0.13	2.0	1.3×10^{-3}	1.9×10^{2}

[a] n.a. = not applicable.

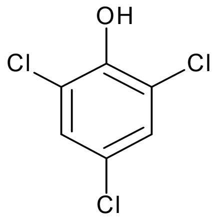
Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), shows that at all sampling occasions and locations, the concentration of 2,4,5 trichlorophenol in water was below detection limits (0.02 µg/L).

3.5 2,4,6-trichlorophenol

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

3.5.1.1 Identity

Table 31. Identification of 2,4,6-trichlorophenol.

Chemical name	2,4,6-trichlorophenol
Product/trade name	Dowicide 2S Omal Phanchlor TCP 2,4,6-T
CAS number	88-06-2
EC number	201-795-9
Annex I Index number	604-018-00-5
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc(c(cc(c1)Cl)Cl)c1Cl

3.5.1.2 Physico-chemical properties

Table 32. Physico-chemical properties of 2,4,6-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**434**	25 ºC; pH 5.1; recommended by reference	Mackay et al., 2000
		800	25 ºC	Muller, 2008; EC, 2000
		121	EpiWin	US EPA, 2007
pK_a	[-]	7.42	Recommended by reference	Mackay et al., 2000
		6.21	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	**3.69**	Recommended by reference	Mackay et al., 2000
		3.69	MlogP (recommended by reference)	BioByte, 2006
		3.39	ClogP (calculated)	BioByte, 2006
		3.45	EpiWin	US EPA, 2007
log K_{OC}	[-]	**2.78**	Geometric mean from cited values	Mackay et al., 2000
		3.22	Calculated using log K_{OW} = 3.69 (QSAR for phenols)	According to Sabljic et al., 1995

Parameter	Unit	Value	Remark	Reference
		3.07	EpiWin	US EPA, 2007
Vapour pressure	[Pa]	1.25	25 ºC, solid, recommended by reference	Mackay et al., 2000
		3.44	25 ºC, liquid, recommended by reference	Mackay et al., 2000
		0.328	EpiWin	US EPA, 2007
Melting point	[°C]	69.5	Recommended by reference	Mackay et al., 2000
		63.8	EpiWin	US EPA, 2007
		68		Muller, 2008
Boiling point	[°C]	246	Recommended by reference	Mackay et al., 2000
		262	EpiWin	US EPA, 2007
		246		Muller, 2008
Henry's law constant	[Pa.m^3/mol]	0.57	Calculated by Mackay	Mackay et al., 2000
		0.54	EpiWin	US EPA, 2007

3.5.1.3 Behaviour in the environment

Table 33. Selected environmental properties of 2,4,6-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]	No hydrolysis		Mackay et al., 2000
Photolysis half-life	DT50 [hr]	1.2-96	Various references	Mackay et al., 2000
Readily biodegradable		Unknown		
Degradability	DT50 [d]	7-65	Seawater; river water; Various references	Mackay et al., 2000
Relevant metabolites		Unknown		

Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.5.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for 2,4,6-trichlorophenol is given in Table 34. Detailed bioaccumulation data for 2,4,6-trichlorophenol are tabulated in Appendix 1.

Table 34. Overview of bioaccumulation data for 2,4,6-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	690		Carlberg et al., 1986
BCF (mussel)	[L/kg]	52	Geometric mean of BCFs determined at various exposure conditions	Makela et al., 1991
BMF	[kg/kg]	1	Default value for compounds with BCF < 2000 L/kg.	

3.5.1.5 Human toxicological treshold limits and carcinogenicity

2,4,6-trichlorophenol is classified as a carcinogenic compound. 2,4,6-trichlorophenol has the following R-phrases relating to human toxicolgy: R22; R36/38; R40; R50/53. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 $\mu g/kg_{bw}$/day (U.S. EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.5.2 Trigger values

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

Table 35. 2,4,6-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	1.78	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.5.1.2
BCF	690	[L/kg]		3.5.1.4
BMF	1	[kg/kg]		3.5.1.4
Log K_{OW}	3.69	[-]		3.5.1.2
R-phrases	R22, R36/38, R40, R50/53	[-]		3.5.1.5
A1 value	1	[µg/L]	Mandatory for phenols	
DW standard	-	[µg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 2,4,6-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 2,4,6-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 2,4,6-trichlorophenol has a BCF ≥ 100 L/kg; assessment of secondary poisoning is triggered.
- 2,4,6-trichlorophenol is a carcinogenic (R40). Furthermore, 2,4,6-chlorophenol has a BCF > 100 L/kg combined with an R22 classification. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.
- For 2,4,6-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 µg/L for phenols applies.

3.5.3 Aquatic toxicity data

3.5.3.1 Toxicity data

An overview of the selected toxicity data for 2,4,6-trichlorophenol is given in Table 36 for freshwater. Marine toxicity data are given in Table 37. Detailed toxicity data for 2,4,6-trichlorophenol are tabulated in Appendix 2.

Table 36. 2,4,6-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a] Taxonomic group	NOEC/EC10 (mg/L)	Acute[a] Taxonomic group	L(E)C50 (mg/L)
Algae	0.33[b]	Bacteria	240
Cyanobacteria	**0.17**	Bacteria	15
Rotifera	0.42	Bacteria	28[f]
Crustacea	0.50	Bacteria	5.1[g]
Insecta	0.59[c]	Bacteria	43
Pisces	1.43[d]	Algae	10
Pisces	0.97[e]	Algae	3.5
		Algae	5.6
		Protozoa	2.0
		Protozoa	4.1[h]
		Macrophyta	0.50[i]
		Fungi	11
		Platyhelmintes	7.1[j]
		Mollusca	5.5
		Annelida	1.4
		Crustacea	2.3[k]
		Crustacea	0.56
		Crustacea	0.50[l]
		Insecta	47
		Pisces	10
		Pisces	0.58[m]
		Pisces	2.2[n]
		Pisces	**0.36[o]**
		Pisces	2.4[p]
		Pisces	0.65[q]
		Pisces	1.5[r]
		Pisces	4.2[s]
		Pisces	0.88[t]
		Pisces	1.1
		Pisces	3.7
		Amphibia	1.2

[a] For detailed information see Appendix 2. Bold values are used for ERL-derivation.
[b] Preferred endpoint, parameter growth rate for *Scenedesmus subspicatus*.
[c] Geometric mean of 0.39, 0.92, and 0.56 mg/L; parameter adult survival for *Paratanytarsus partenogenetica*.
[d] Most sensitive endpoint, parameter mortality for *Jordanella floridae*.
[e] Most sensitive endpoint, parameter survival and growth for *Pimephales promelas*.
[f] Most sensitive endpoint, parameter bioluminescence for *Escherichia coli.*
[g] Most sensitive pH (7.1), parameter bioluminescence for *Pseudomonas fluorescens*.
[h] Geometric mean of 7.68, 3.00, 3.94, and 3.10 mg/L, parameter population growth for *Tetrahymena pyriformis*.
[i] Most sensitive endpoint, parameter yield (dry weight) for *Lemna minor* .
[j] Most sensitive endpoint, head regeneration for *Dugesia japonica*.
[k] Geometric mean of 4.00 and 1.74 mg/L, parameter mortality/immobility for *Ceriodaphnia dubia.*

[l] most sensitive pH (6.0-6.5), geometric mean of 0.75 and 0.33 mg/L, parameter mortality/immobilisation for *Daphnia magna*.
[m] Most sensitive exposure duration (96 h), parameter mortality for *Danio rerio*.
[n] Geometric mean of 2.26 and 2.21 mg/L, parameter mortality for *Jordanella floridae*.
[o] Geometric mean of 0.32 and 0.41 mg/L, paramter mortality for *Lepomis macrochirus*.
[p] Geometric mean of 3.0 and 1.9 mg/L, parameter mortality for *Leuciscus idus*.
[q] Geometric mean of 0.57 and 0.73 mg/L, parameter mortality for *Oncorhynchus mykiss*.
[r] Geometric mean of 1.50 and 1.51 mg/L, parameter mortality for *Oryzias latipes*.
[s] Geometric mean of 9.7, 8.6, 4.55, 4.16, 0.6, and 2.74 mg/L, most relevant exposure duration (96 h), parameter mortality for *Pimephales promelas*.
[t] Most sensitive pH (6.0), parameter mortality for *Poecilia reticulata*.

Table 37. 2,4,6-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a]		Acute [a]	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
Bacteria	0.054	Bacteria	11[b]
Algae	0.28	Algae	4
		Algae	0.5
		Algae	10
		Algae	8
		Algae	4
		Crustacea	1.2[c]
		Pisces	2.3
		Pisces	1.4

[a] For detailed information see Appendix 2.
[b] most relevant exposure duration (15 to 30 min.), geometric mean of 12.7, 7.7, 10.4, 14.7, 4.3, 23, 6.7, 22.6, and 7.1 mg/L, parameter bioluminescence for *Vibrio fischeri*.
[c] most sensitive life-stage (molting adults), parameter mortality for *Palaemonetes pugio*.

3.5.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 2,4,6-trichlorophenol are combined.

3.5.4 Derivation of Environmental Risk Limits

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

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

Acute toxicity data are available for 11 taxonomic groups, amongst which algae, crustacea (*Daphnia*) and fish. Thus, the base set is complete. Chronic toxicity data are available for algae, cyanobacteria, rotifera, insecta, crustacea and fish.

Chronic data for bacteria may not be used for MPC derivation (Lepper, 2005), but are included in the aggregated data table because it can be used for SRC derivation. Cyanobacteria are an exception to this. Thus, the lowest NOEC for MPC derivation is 0.17 mg/L for the cyanobacteria *Anabaena* sp.

For the freshwater environment, an assessment factor of 10 can be used on the lowest NOEC, which results in an $MPC_{eco, water}$ of 0.17 / 10 = 1.7 × 10^{-2} mg/L = 17 µg/L.

No chronic toxicity data are available for specific marine taxa. Thus, with an assessment factor of 100 the $MPC_{eco, marine}$ becomes 0.17 / 100 = 1.7 × 10^{-3} mg/L = 1.7 µg/L.

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

2,4,6-trichlorophenol has a BCF ≥ 100 L/kg, thus assessment of secondary poisoning is triggered.

The lowest MPC_{oral} is 3.3 mg/kg (see table Table 38) . Subsequently, the $MPC_{sp, water}$ can be calculated using a BCF of 690 L/kg and a BMF of 1 kg/kg (section 3.5.1.4) and becomes
3.3 / (690 × 1) = 4.8 × 10^{-3} mg/L = 4.8 µg/L.

Table 38. 2,4,6-trichlorophenol: selected mammal data for ERL derivation.

Species[a]	Exposure time	Criterion	Effect concentration (mg/kg diet)	Assessment factor	MPC_{oral} (mg/kg diet)
Rat	2 weeks pre-mating and through gestation	NOAEL	1000	300	3.33

[a] For detailed information see Appendix 3.
[b] based on a NOAEL of 100 mg/kg_{bw}/day with a conversion factor of 10.

For the marine environment, an extra biomagnification factor should be used. But since this factor is 1 by default for compounds with log K_{OW} < 4.5, the $MPC_{sp, marine}$ equals the $MPC_{sp, water}$ and is also 4.8 µg/L.

$MPC_{hh food, water}$

Derivation of $MPC_{hh food, water}$ for 2,4,6-trichlorophenol is triggered (Table 35). With an ADI of 0.003 mg/kg_{bw}/d for phenols, a BCF of 690 L/kg and a BMF of 1 kg/kg (section 3.5.1.4) , the $MPC_{hh food}$ becomes (0.1 × 0.003 × 70) / 0.115 = 0.183 mg/L. Subsequently, the $MPC_{hh food, water}$ and $MPC_{hh food, marine}$ become 0.183 / (690 × 1) = 0.00026 mg/L = 0.26 µg/L.

$MPC_{dw, water}$

The $MPC_{dw, water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC.

For the freshwater environment, the lowest MPC value is the value for human consumption of fishery products of 0.26 µg/L. Thus, the overall MPC_{water} is 0.26 µg/L.

For the marine environment, the lowest MPC value is the value for direct human consumption of fishery products of 0.26 µg/L. Thus, the overall MPC_{marine} is 0.26 µg/L.

3.5.4.2 Derivation of MAC_{eco}

The base-set for acute data is complete. With toxicity data available for 12 different taxa (bacteria, algae, protozoa, macrophyta, fungi, platyhelminthes, mollusca, annelida, crustacea, fish, amphibia), enough data are present to perform an SSD. This results in a HC5 of 0.32 mg/L (95% confidence interval: 0.16 – 0.53 mg/L) with a goodness of fit that is accepted at all significance levels (see Figure 1). According to Lepper (2005), a default assessment factor of 10 should be used on the results of an SSD for acute data. There is no reason to change the assessment factor and thus the MAC_{eco} becomes 0.32 / 10 = 0.032 mg/L = 32 µg/L.

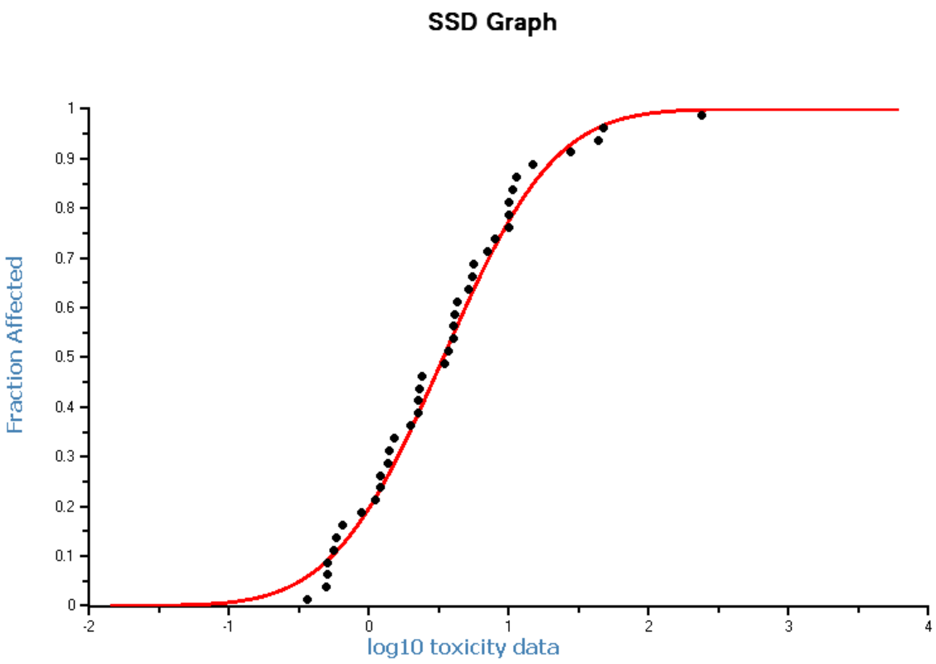


Figure 1. SSD graph for acute toxicity data of 2,4,6-trichlorophenol.

Regarding the assessment factor approach, the BCF is higher than 100 L/kg, the compound has a non-specific mode of action, and the interspecies variation is high (more than a factor of 100 between the highest and the lowest LC50). However, the somewhat higher ratio between the highest and lowest LC50 is mainly caused by the vast amount of data present; due to the amount of data, the difference between the highest and lowest LC50 increases. Moreover, due to this amount of data present, it can be assumed with high probability that all sensitive taxa are reflected in the dataset and thus, an assessment factor of 100 seems justified. Using the lowest L(E)C50 value (0.36 mg/L for *Danio rerio*), the MAC_{eco} becomes 0.36 / 100 = 0.0036 mg/L = 3.6 µg/L.

Because of the quality of the SSD (high goodness of fit), the small 95% confidence interval for the HC5 and the high number of taxa present in the acute dataset, the final $MAC_{eco,\ water}$ is based on the results of the SSD approach and becomes 32 µg/L.

For the marine environment, an additional assessment factor of 10 should be used because no specific marine taxa are present in the dataset. Thus, the $MAC_{eco,\ marine}$ becomes 3.2 µg/L.

3.5.4.3 Derivation of NC

The NC is derived by dividing the final MPC by a factor of 100.

NC_{water} = 2.6 × 10^{-3} µg/L.
NC_{marine} = 2.6 × 10^{-3} µg/L.

3.5.4.4 Derivation of SRC_{eco}

The geometric mean of all chronic data is 0.37 mg/L. These data are normally distributed (at all levels using the Anderson-Darling test for normality). Because more than three NOECs are available, no comparison has to be made with the geometric mean of the acute data. Thus, the $SRC_{eco,\ water}$ and $SRC_{eco,\ marine}$ are set at 0.37 mg/L = 370 µg/L.

3.5.5 Sediment compartment

The log $K_{p\ susp\text{-}water}$ of 2,4,6-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.5.6 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 39.

Table 39. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values for 2,4,6-trichlorophenol (in µg/L).

ERL	Unit	MPC	MAC_{eco}	NC	SRC_{eco}
Freshwater	µg/L	0.26	32	2.6 × 10^{-3}	3.7× 10^{2}
Drinking water	µg/L	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	µg/L	0.26	3.2	2.6 × 10^{-3}	3.7× 10^{2}

[a] n.a. = not applicable.

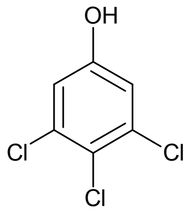
Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of 2,4,6 trichlorophenol in water was below detection limits (0.02 µg/L).

3.6 3,4,5-trichlorophenol

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

3.6.1.1 Identity

Table 40. Identification of 3,4,5-trichlorophenol.

Chemical name	3,4,5-trichlorophenol
CAS number	609-19-8
EC number	210-183-0
Structural formula	
Molecular formula	$C_6H_2Cl_3OH$
SMILES code	Oc1cc(Cl)c(Cl)c(Cl)c1

3.6.1.2 Physico-chemical properties

Table 41. Physico-chemical properties of 3,4,5-trichlorophenol. Bold values are used for ERL derivation.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	197.45		
Water solubility	[mg/L]	**64.5**	EpiWin	US EPA, 2007
pK_a	[-]	7.74	Recommended by reference	Mackay et al., 2000
		7.81	Recommended by reference	BioByte, 2006
log K_{OW}	[-]	4.3	Recommended by reference	Mackay et al., 2000
		4.01	MlogP (recommended by reference)	BioByte, 2006
		3.81	ClogP (calculated)	BioByte, 2006
		3.45	EpiWin	US EPA, 2007
log K_{OC}	[-]	**3.43**	Calculated using log K_{OW} = 4.01 (QSAR for phenols)	According to Sabljic et al., 1995
		3.07	EpiWin	US EPA, 2007
Vapour pressure	[Pa]	0.328	EpiWin	US EPA, 2007
Melting point	[°C]	101	Recommended by reference	Mackay et al., 2000
		63.8	EpiWin	US EPA, 2007
		101		Muller, 2008
Boiling point	[°C]	262	EpiWin	US EPA, 2007
		275		Muller, 2008
Henry's law constant	[Pa.m^3/mol]	1.00	EpiWin	US EPA, 2007

3.6.1.3 Behaviour in the environment

No specific data on environmental behaviour is available for 3,4,5-trichlorophenol. Biodegradation of chlorophenols must be induced, because the antimicrobial activities of these products require that the bacteria adapt. Biodegradation is rapid when adapted bacteria are present (Muller, 2008).

3.6.1.4 Bioconcentration and biomagnification

Bioaccumulation data for 3,4,5-trichlorophenol are tabulated inTable 42. No experimental bioaccumulation data were available.

Table 42. Overview of bioaccumulation data for 3,4,5-trichlorophenol.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	511	Calculated using log K_{OW} = 4.01	According to Veith et al., 1979
BMF	[kg/kg]	1	Default value for compounds with log K_{OW} > 4.5	

3.6.1.5 Human toxicological treshold limits and carcinogenicity

3,4,5-trichlorophenol has the following R-classification: R36/37/38. Polychlorophenols in general are classified as being possibly carcinogenic to humans (group 2B) by the IARC (IARC, 1999). The TDI for 2,4-dichlorophenol of 3 μg/kg_{bw}/day (U.S. EPA, 1986) was considered to be valid for all mono-, di-, tri-, and tetrachlorophenol compounds (Baars et al., 2001).

3.6.2 Trigger values

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

Table 43. 3,4,5-trichlorophenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp\text{-}water}$	2.43	[-]	$K_{OC} \times f_{OC,susp}$ [1]	K_{OC}: 3.6.1.2
BCF	511	[L/kg]		3.6.1.4
BMF	1	[kg/kg]		3.6.1.4
Log K_{OW}	4.01	[-]		3.6.1.2
R-phrases	R36/37/38	[-]		3.6.1.5
A1 value	1	[μg/L]	Mandatory for phenols	
DW standard	-	[μg/L]		

1 $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} (European Commission (Joint Research Centre), 2003).

- 3,4,5-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{sediment}$ is not triggered.
- 3,4,5-trichlorophenol has a log $K_{p,\ susp\text{-}water}$ < 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 3,4,5-trichlorophenol has a log $K_{OW} \geq$ 3; assessment of secondary poisoning is triggered.
- 3,4,5-trichlorophenol does not have any relevant R-classifications, but is classified as a possible carcinogenic. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) has to be derived.
- For 3,4,5-trichlorophenol, no compound-specific A1 value or Drinking Water standard value is available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, the general mandatory A1 value of 1 μg/L for phenols applies.

3.6.3 Aquatic toxicity data

3.6.3.1 Toxicity data

An overview of the selected toxicity data for 3,4,5-trichlorophenol is given in Table 44 for freshwater and in Table 45 for the marine environment. Detailed toxicity data for 3,4,5-trichlorophenol are tabulated in Appendix 2.

Table 44. 3,4,5-trichlorophenol: selected freshwater toxicity data for ERL derivation.

Chronic[a]		**Acute**[a]	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
Algae	0.15	Bacteria	5.0
Algae	**0.06**	Bacteria	0.87
Algae	0.18	Bacteria	1.9
		Macrophyta	0.32
		Crustacea	0.39
		Crustacea	0.68[b]
		Crustacea	0.40
		Pisces	**0.20**[c]
		Pisces	1.1[d]

a For detailed information see Appendix 2. Bold values are used for ERL-derivation.
b Preferred exposure duration (48 h), parameter mortality/immobility for *Daphnia magna.*
c Most sensitive life stage (larvae), parameter mortality for *Danio rerio.*
d Most sensitive pH (6.1), parameter mortality for *Poecilia reticulata.*

Table 45. 3,4,5-trichlorophenol: selected marine toxicity data for ERL derivation.

Chronic [a]		**Acute** [a]	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
No data		Bacteria	0.38[b]
		Pisces	2.31

a For detailed information see Appendix 2.
b Geometric mean of 0.36, 0.34, 0.39, and 0.47 mg/L, parameter bioluminescence for *Vibrio fischeri.*

3.6.3.2 Treatment of fresh- and saltwater toxicity data

Following Lepper (2005), freshwater and marine datasets can be combined if it cannot be shown that the sensitivity of marine species is different from that of freshwater species. Thus, freshwater and marine datasets for 3,4,5-trichlorophenol are combined.

3.6.4 Derivation of Environmental Risk Limits

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

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

Although no acute toxicity data for algae are present, due to the presence of macrophytes in the dataset (another primary producer and also sensitive to uncoupling of the electron transport) it can be assumed that the acute base set is present. However, chronic data are only available for algae. Algae are not present in the acute dataset, and thus the NOEC is not from the species with the lowest LC50. An assessment factor of 1000 should then be used on the lowest L(E)C50 (0.20 mg/L for the fish

Danio rerio), assuming that the EC50 values for the algae *Nitzschia* would not be lower than this value. Thus, the $MPC_{eco, water}$ becomes 0.20 / 1000 = 2.0×10^{-4} mg/L = 0.20 µg/L.

No data are available for specific marine species, thus for the $MPC_{eco, marine}$, an assessment factor of 10000 should be used on the lowest L(E)C50 and the $MPC_{eco, marine}$ becomes
0.20 / 10000 = 2.0×10^{-5} mg/L = 2.0×10^{-2} µg/L.

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

3,4,5-trichlorophenol has a log $K_{OW} \geq 3$, thus assessment of secondary poisoning is triggered. No bird or mammal data for 2,4,5-trichlorophenol are available. Regarding the other trichlorophenols, only bird and mammal data are available for 2,4,6-trichlorophenol. Thus, to obtain an *indication* on the relevance of the exposure route, the lowest MPC_{oral} (3.3 mg/kg) for 2,4,6-trichlorophenol is used (see section 3.5.4.1). Subsequently, the $MPC_{sp, water}$ can be calculated using a BCF of 511 L/kg and a BMF of 1 kg/kg (section 3.6.1.4) and becomes 3.3 / (511 × 1) = 6.5×10^{-3} mg/L = 6.5 µg/L.

$MPC_{hh food, water}$

Derivation of $MPC_{hh food, water}$ for 3,4,5-trichlorophenol is triggered (Table 43). With an ADI of 0.003 mg/kg_{bw}/d for phenols, a BCF of 511 L/kg and a BMF of 1 kg/kg (section 3.6.1.4) , the $MPC_{hh food}$ becomes (0.1 × 0.003 × 70) / 0.115 = 0.183 mg/L. Subsequently, the $MPC_{hh food, water}$ and $MPC_{hh food, marine}$ become 0.183 / (511 × 1) = 0.00036 mg/L = 0.36 µg/L.

$MPC_{dw, water}$

The $MPC_{dw, water}$ is 1 µg/L according to the general A1 value for phenols.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC.

For the freshwater environment, the lowest MPC value is the value for direct ecotoxicity of 0.20 µg/L. Thus, the overall MPC_{water} is 0.20 µg/L.

For the marine environment, the lowest MPC value is the value for direct ecotoxicity of 2.0×10^{-2} µg/L. Thus, the overall MPC_{marine} is 2.0×10^{-2} µg/L.

3.6.4.2 Derivation of MAC_{eco}

Assuming the base set is complete (with macrophytes instead of algae), a MAC_{eco} can be derived. The compound has potential to bioaccumulate, the mode of action is non-specific and interspecies variation is low. Thus, an assessment factor of 100 can be used on the lowest acute LC50 (0.20 mg/L for the fish *Danio rerio*), and the $MAC_{eco, water}$ becomes 0.20 / 100 = 0.0020 mg/L = 2.0 µg/L.

The $MAC_{eco, marine}$ should be derived with an additional assessment factor of 10 (no specific marine taxa present) and becomes 0.20/ 1000 = 0.000020 mg/L = 0.20 µg/L.

3.6.4.3 Derivation of NC

The NC is derived by dividing the final MPC by a factor of 100.

NC_{water} = 2.0×10^{-3} µg/L.
NC_{marine} = 2.0×10^{-4} µg/L.

3.6.4.4 Derivation of SRC_{eco}

NOECs are available for only one taxon, which means that the geometric mean of all chronic data should be compared to the geometric mean of all acute data. The geometric mean of all NOECs is 0.12 mg/L, the geometric mean of all LC50s is 0.76 mg/L (accepted at all levels using the Anderson-Darling test for normality). Because the geometric mean of the acute data divided by 10 is smaller than the geometric mean of the chronic data, the SRC_{eco} should be derived based on the acute data with an assessment factor of 10 and becomes 0.76 / 10 = 0.076 mg/L = 76 µg/L.

3.6.5 Sediment compartment

The log $K_{p,\ susp\text{-}water}$ of 3,4,5-trichlorophenol is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.6.6 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 46.

Table 46. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values for 3,4,5-trichlorophenol (in µg/L).

ERL	Unit	MPC	MAC_{eco}	NC	SRC_{eco}
Freshwater	µg/L	0.20	2.0	2.0×10^{-3}	76
Drinking water	µg/L	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	µg/L	2.0×10^{-2}	0.20	2.0×10^{-4}	76

[a] n.a. = not applicable.

Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of 3,4,5 trichlorophenol in water was below detection limits (0.02 µg/L).

rivm

4 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 trichlorophenols in water. No risk limits were derived for the sediment compartment because the trigger values to derive such risk limits were not reached.

Please note that due to the mode of action of the trichlorophenols (narcosis), and the fact that these compounds often occur together, the use of the toxic unit approach is recommended. The toxic unit approach assumes that compounds that act similar, have concentration additive toxicity. This means that the sum of the ratio between measured concentration and risk limits for all trichlorophenols should not exceed 1.

The ERLs that were obtained are summarised in the table below.

Table 47. Derived MPC, MAC_{eco}, NC, and SRC_{eco} values (in µg/L).

	MPC	MAC_{eco}	NC	SRC_{eco}
2,3,4-trichlorophenol				
Freshwater	0.54	12	5.4×10^{-3}	2.6×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	0.12	1.2	1.2×10^{-3}	2.6×10^{2}
2,3,5-trichlorophenol				
Freshwater	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
2,3,6-trichlorophenol				
Freshwater	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	n.d.[b]	n.d.[b]	n.d.[b]	n.d.[b]
2,4,5-trichlorophenol				
Freshwater	0.13	2.6	1.3×10^{-3}	1.9×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	0.13	2.0	1.3×10^{-3}	1.9×10^{2}
2,4,6-trichlorophenol				
Freshwater	0.26	32	2.6×10^{-3}	3.7×10^{2}
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	0.26	3.2	2.6×10^{-3}	3.7×10^{2}
3,4,5-trichlorophenol				
Freshwater	0.20	2.0	2.0×10^{-3}	76
Drinking water	1	n.a.[a]	n.a.[a]	n.a.[a]
Marine water	2.0×10^{-2}	0.20	2.0×10^{-4}	76

[a] n.a. = not applicable.

[b] n.d. = not derived due to a lack of data.

rivm

References

Baars AJ, Theelen RMC, Janssen PJCM, Hesse JM, van Apeldoorn ME, Meijerink MCM, Verdam L, Zeilmaker MJ. 2001. Re-evaluation of human-toxicological maximum permissible risk levels. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report number 711701025.

BioByte. 2006. BioLoom [computer program]. version 1.0 (ClogP 4.0). Claremont, CA, USA: BioByte Corporation.

Call DJ, Brooke LT, Lu P-Y. 1980. Uptake, elimination and metabolism of three phenols by fathead minnows. Arch Environ Contam Toxicol 9: 699-714.

Carlberg GE, Martinsen K, Kringstad A, Gjessing E, Grande M, Källqvist, SkÍre JU. 1986. Influence of aquatic humus on the biovailability of chlorinated micropollutants in atlantic salmon. Arch Environ Contam Toxicol 15: 543-548.

European Commission (European Chemical Bureau). 2000. IUCLID (International Uniform Chemical Information Database) on CD-ROM. European Chemicals Bureau, Ispra, Italy.

European Commission (Joint Research Centre). 2003. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/9/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Part II. Ispra, Italy: European Chemicals Bureau, Institute for Health and Consumer Protection. Report no. EUR 20418 EN/2.

IARC. 1999. Monographs on the Evaluation of Carcinogenic Risks to Humans. Volume 71. Re-Evaluation of Some Organic Chemicals, Hydrazine and Hydrogen Peroxide. International Agency for Research on Cancer, Lyon, France.

Lepper P. 2005. Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC). 15 September 2005 (unveröffentlicht) ed. Schmallenberg, Germany: Fraunhofer-Institute Molecular Biology and Applied Ecology.

Mackay D, Shiu WY, Ma KC. 2000. Physical-chemical properties and environmental fate. Handbook. Chapman and Hall/ CRCnetBase.

Makela TP, Petanen T, Kukkonen J, Oikari OJ. 1991. Accumulation and depuration of chloronated phenolics in the freshwater mussel (Anodonta anatina L.). Ecotoxicol Environ Saf 22: 153-163.

Moermond CTA, Heugens EHW. 2009a. Environmental risk limits for monochlorophenols, 4-chloro-3-methyl-phenol and aminochlorophenol. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 601714006.

Moermond CTA, Heugens EHW. 2009b. Environmental risk limits for 2,4-dichlorophenol. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 601714007.

Muller F, 2008. Chlorophenols. In: Ullmann's Encyclopedia of Industrial Chemistry. John Wiley & Sons, Inc. (http://mrw.interscience.wiley.com/emrw/3527-306730/home/; feb 08).

National Pollutant Inventory. 2005. Department of the environment, water, heritage and the arts, Australia. (http://www.npi.gov.au/database/substance-info/profiles/90.html#common; feb 08).

Sabljic A, Güsten H, Verhaar H, Hermens J. 1995. QSAR modelling of soil sorption. Improvements and systematics of log Koc versus log Kow correlations. Chemosphere 31: 4489-4514.

US EPA.1986. Health Effects Assessment for Selected Chlorinated Phenols. Prepared by the Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH for the Office of Emergency and Remedial Response, Washington, DC.

US EPA. 2007. EPI Suite™ [computer program]. version 3.2. Washington, DC, U.S.A.: U.S. Environmental Protection Agency (EPA) Office of Pollution Prevention Toxics and Syracuse

Research Company (SRC).
Van Vlaardingen PLA, Verbruggen EMJ. 2007. Guidance for the derivation of environmental risk limits within the framework of the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS). Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 601782001.
Veith GD, DeFoe DL, Bergstedt BV. 1979. Measuring and estimating the bioconcentration factor of chemicals in fish. J. Fish Res.; 36, 1040-1048.

Appendix 1. Information on bioconcentration

Table A1.1 Bioconcentration data for 2,3,5-trichlorophenol.

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pisces																
Salmo trutta	4.5 g	97	GC-ECD	S				5	24 h	4	12	LBB	Cbiota/Cw	3	1	Hattula et al., 1981

Notes
1 Lethal body burdens; static system; maximum of 100 ml ethanol/l

Table A1.2 Bioconcentration data for 2,4,5-trichlorophenol.

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Annelida																
Nephelopsis obscura	field collected, 0.826 ± 0.214g		deriv GC-ECD	R	rw	7	60	4	7 d	0.01	593	whole body ww	Cbiota/Cw	2	1,6	Hall and Jacob, 1988
Nephelopsis obscura	field collected, 0.669 ± 0.160g		deriv GC-ECD	R	rw	7	60	12	7 d	0.01	969	whole body ww	Cbiota/Cw	2	1,6	Hall and Jacob, 1988
Nephelopsis obscura	field collected, 0.845 ± 0.271g		deriv GC-ECD	R	rw	7	60	22	7 d	0.01	1948	whole body ww	Cbiota/Cw	3	1,7	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.01	60	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.02	72	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.03	100	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 0.079±0.006 g		deriv GC-ECD	R	rw	5	60	4	24 h	0.01	115	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 0.079±0.006 g		deriv GC-ECD	R	rw	7.5	60	4	24 h	0.01	51	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 0.079±0.006 g		deriv GC-ECD	R	rw	9.2	60	4	24 h	0.01	13	whole body ww	Cbiota/Cw	3	1,8	Hall and Jacob, 1988
Unspecified											1862		Cbiota/Cw	4	2	Klamer and Beekman, 1995
Crustacea																
Palaemonetes pugio	intermoult adults; field-collected from clean site; 25 mm		LSC		nw (filtered sea water)			20	12 h	1	32	whole body ww	Cbiota/Cw; total 14C	3	9	Rao et al., 1981
Palaemonetes pugio	newly moulted (stage A), field-collected from clean site; 25 mm		LSC		nw (filtered sea water)			20	1 h	1	32	whole body ww	Cbiota/Cw; total 14C	3	10	Rao et al., 1981
Mollusca																
Pisidium amnicum	field-collected; 5.1-7.3 mm shell length		LSC	S	am	6.5	50	15	72 h	0.0045-0.0054	167	soft tissue ww	k1/k2	3	3,11	Heinonen et al., 2000
Pisidium amnicum	field-collected; 5.1-7.3 mm shell length		LSC	S	am	6.5	50	15	72 h	0.0045-0.0054	172	soft tissue ww	Cbiota/Cw	3	3,11	Heinonen et al., 2000

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pisidium amnicum	field-collected; 5.1-7.3 mm shell length; 7.2% lipids		LSC	S	am	6.5	50	15	72 h	0.0045-0.0054	313	soft tissue ww	k1/k2	3	3,11	Heinonen et al., 2000
Pisidium amnicum	field-collected; 5.1-7.3 mm shell length; 7.2% lipids		LSC	S	am	6.5	50	15	72 h	0.0045-0.0054	318	soft tissue ww	Cbiota/Cw	3	3,11	Heinonen et al., 2000
Pisidium amnicum	field-collected; 5.1-8.2 mm shell length; 8.7% lipids		LSC	S	am	6.5	50	4	144 h	0.0045-0.0054	233	soft tissue ww	k1/k2	3	3,11	Heinonen et al., 2000
Pisidium amnicum	field-collected; 5.1-8.2 mm shell length; 8.7% lipids		LSC	S	am	6.5	50	4	144 h	0.0045-0.0054	236	soft tissue ww	Cbiota/Cw	3	3,11	Heinonen et al., 2000
Sphaerium corneum	field collected; 9-11 mm		LSC	S	am	6.5	50	20	168 h	0.05	115-139	soft tissue ww	Cbiota/Cw	3	11	Heinonen et al., 1997
Pisces																
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	6		20-21	5 h	0.3	61	whole body	Cbiota/Cw	3	12	Kishino and Kobayashi, 1995
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	8		20-21	5 h	0.3	22	whole body	Cbiota/Cw	3	12	Kishino and Kobayashi, 1995
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	10		20-21	5 h	0.3	1.8	whole body	Cbiota/Cw	3	12	Kishino and Kobayashi, 1995
Carassius auratus	2 g		colorimetric	R				20	12- 24 h	1.8	62	whole body	Cbiota/Cw	3	13	Kobayashi et al., 1979
Pimephales promelas									28 d		1905			4	4	Call and Brook, 1977 in Veith et al., 1979a
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0048	1493	whole body	equilibrium Cbiota/Cw	1	14	Call et al., 1980
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0048	**1414**	whole body	non-linear regression	1	5,15	Call et al., 1980
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0048	395	whole body	k1/k2 independant	3	5,16	Call et al., 1980

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC + TLC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0493	**1414**	whole body	equilibrium Cbiota/Cw	1	17	Call et al., 1980
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC + TLC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0493	**1414**	whole body	non-linear regression	1	5,17	Call et al., 1980
Pimephales promelas	28 -42 d old; 0.1-0.15 g 4.1% lipid; 0.22-0.26 g 5.3% lipid; 0.4-0.49 g 8.2% lipid	98	LSC + TLC	F	nw	7.36-7.62	40.0-43.2	22.0±0.6	28 d	0.0493	520	whole body	k1/k2 indepen-dant	3	5,18	Call et al., 1980

Notes:

1 Analyses indicated that there was no significant volatilization or photodegradation of the chlorophenols after a 24h exposure period.
2 Review; mentioned in review that metabolic transformation does not occur.
3 Result originally reported in dw; recalculated into ww using reporte dw/www of 0.0925.
4 Review.
5 Number used taken from text, with calculation of k1 including depuration.
6 3 leaches per timepoint; steady state was reached within 5 days
7 3 leaches per timepoint; steady state wasnot reached during the experiment
8 only 1 leech used per experiment. May have been pre-exposed but probably not
9 Exposure duration too short; toxic effects possible at this concentration
10 Exposure duration too short; toxic effects possible at this concentration
11 total 14C
12 Exposure duration is short, equilbrium might not be fully reached; aquaeous concentration presumably not measured
13 Exposure duration is short; aquaeous concentration presumably not measured
14 Mean measured concentrations very close to nominal concentrations. Reported BCF is 1900 l/kg, based on total 14C amount. At end of uptake phase % parent is 78.6 in the high concentration, thus parent BCF is 1493
15 Mean measured concentrations very close to nominal concentrations. Methanol used as solvent at 0.1 ml/l. Reported BCF is 1800 l/kg, based on total 14C amount. At end of uptake phase % parent is 78.6 in the high concentration, thus parent BCF is 1493.
16 Mean measured concentrations very close to nominal concentrations. Methanol used as solvent at 0.1 ml/l. Reported BCF is 503 l/kg, based on total 14C amount. At end of uptake phase % parent is 78.6 in the high concentration. Invalid due to biphasic elimination because of LSC instead of analysis of parent compound and erroneous low k1 due to metabolism.
17 Mean measured concentrations very close to nominal concentrations. Methanol used as solvent at 0.1 ml/l. Reported BCF is 1800 l/kg, based on total 14C amount. At end of uptake phase % parent is 78.6, thus parent BCF is 1415
18 Mean measured concentrations very close to nominal concentrations. Methanol used as solvent at 0.1 ml/l. Reported BCF is 662 l/kg, based on total 14C amount. At end of uptake phase % parent is 78.6. Invalid due to biphasic elimination because of LSC instead of analysis of parent compound and erroneous low k1 due to metabolism.

Table A1.3 Bioconcentration data for 2,4,6-trichlorophenol.

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Algae																
Chlorella fusca var. Vacuolate	0.1 mg dw/ml	99	LSC	S	am			20-25	24 h	0.05	51	whole body ww	Cbiota/Cw; 14C	2		Freitag et al., 1982; Geyer et al., 1984
Chlorella fusca var. Vacuolate	0.1 mg dw/ml		LSC	S	am			20-25	24 h	0.05	580	whole body dw	Cbiota/Cw+N5; 14C+N5	2	1	Korte et al., 1978; Korte, 1990
Annelida																
Nephelopsis obscura	field collected, 0.826 ± 0.214g		deriv GC-ECD	R	rw	7	60	4	7 d	0.01	524	whole body ww	Cbiota/Cw	2	2,7	Hall and Jacob, 1988
Nephelopsis obscura	field collected, 0.669 ± 0.160g		deriv GC-ECD	R	rw	7	60	12	7 d	0.01	869	whole body ww	Cbiota/Cw	2	2,7	Hall and Jacob, 1988
Nephelopsis obscura	field collected, 0.845 ± 0.271g		deriv GC-ECD	R	rw	7	60	22	7 d	0.01	1948	whole body ww	Cbiota/Cw	3	2,8	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.01	58	whole body ww	Cbiota/Cw	3	2,9	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.02	50	whole body ww	Cbiota/Cw	3	2,9	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 1.35±0.37 g		deriv GC-ECD	R	rw	7	60	22	24 h	0.03	79	whole body ww	Cbiota/Cw	3	2,9	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 0.079±0.006 g		deriv GC-ECD	R	rw	5	60	4	24 h	0.01	90	whole body ww	Cbiota/Cw	3	2,9	Hall and Jacob, 1988
Percymoorensis marmorata or Nephelopsis obscura	field collected, 0.079±0.006 g		deriv GC-ECD	R	rw	7.5	60	4	24 h	0.01	57	whole body ww	Cbiota/Cw	3	2,9	Hall and Jacob, 1988
Mollusca																
Not specified	6-10 g													4	10	Makela et al., 1991, in Belfroid et al., 1996
Anodonta anatina	field-collected; 89 mm; 4.9% lipid		deriv GC-ECD	S	ftw	8.0 - 8.2	54	18	10 d	0.02	1130	soft body dw	Cbiota/Cw	4	11	Englund & Heino, 1996
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	R	dtw	7.1±0.2		3	8 d	0.0013	38	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	R	dtw	7.1±0.2		8	8 d	0.00168	38	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	R	dtw	7.1±0.2		13	8 d	0.00141	33	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	R	dtw	7.1±0.2		18	8 d	0.00151	31	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	S	dtw	7.1±0.2		13	8 d	0.00115	125	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	S	dtw	7.1±0.2		13	8 d	0.00463	30	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	S	dtw	7.1±0.2		13	8 d	0.0106	68	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Anodonta anatina	field-collected; 6--8 cm; 6-10 g; 8-12years; 1.5-1.5% lipids	98	GC-ECD	CF	dtw	7.1±0.2		13	4 d	0.00522	141	soft body ww	Cbiota/Cw	3	3,12	Makela et al., 1991
Lymnea stagnalis	0.12 - 1.7 g	99	deriv GLC-ECD	F	dtw	7.0 - 7.3	52.05	18.6 - 20.1	36 d	0.0005	3020	soft body ww	Cbiota/Cw	3	13,14	Virtanen & Hattula, 1982

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness $CaCO_3$ [mg/L]	Temp. [°C]	Exp. time	Exp. concn. [mg/L]	BCF [L/kg]	BCF type	Calculation method	Ri	Notes	Reference
Lymnea stagnalis	0.12 - 1.7 g	99	deriv GLC-ECD	F	dtw	7.0 - 7.3	52.05	18.6 - 20.1	45 d	0.0005	410	soft body ww	Cbiota/Cw	3	13,15	Virtanen & Hattula, 1982
Mytilus edulis	obtained from fish market	ag	GC-MS	R	nw			15	7 d	0.1	29.05	sof tissue body ww	(equilibrium) Cbiota/Cw or kinetic	2	16	Jennings et al, 1996
Pisces																
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	6		20-21	5 h	0.3	160	whole body	Cbiota/Cw	3	17	Kishino and Kobayashi, 1995
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	8		20-21	5 h	0.3	40	whole body	Cbiota/Cw	3	17	Kishino and Kobayashi, 1995
Carassius auratus	2.2 g	100	deriv GC/ECD (not in water)	S	tw	10		20-21	5 h	0.3	1.8	whole body	Cbiota/Cw	3	17	Kishino and Kobayashi, 1995
Carassius auratus	2 g		colorimetric	R				20	12-24 h	10	20	whole body	Cbiota/Cw	3	17	Kobayashi et al., 1979
Leuciscus idus melanotus	1.5 g, 5-6 cm	99	LSC	S	tw/dw		80-85	20-25	3 d	0.03	310	whole body ww	Cbiota/Cw	3	18	Freitag et al., 1982; Freitag et al., 1984
Leuciscus idus melanotus	2 - 5 g		LSC	S	tw/dw		100	23±3	3 d	0.05	250	whole body ww	Cbiota/Cw	3	18	Korte et al., 1978; Korte, 1990; EC, 2000
Oncorhynchus mykiss	eggs		LSC		rw			10	28d	0.2	190	whole body ww	Cbiota/Cw	3	4,19	Freitag et al., 1991
Poecilia reticulata	50 - 350 mg; female	99	deriv GLC-ECD	F	dtw	7.0 - 7.3	52.05 mg CaCO3 /L	18.6 - 20.1	52 d	0.0005	6080	whole body ww	Cbiota/Cw	3	13,20	Virtanen & Hattula, 1982; EC, 2000
Poecilia reticulata	48 - 194 mg; males	99	deriv GLC-ECD	F	dtw	7.0 - 7.3	52.05 mg CaCO3 /L	18.6 - 20.1	52 d	0.0005	3375	whole body ww	Cbiota/Cw	3	13,20	Virtanen & Hattula, 1982; EC, 2000
Salmo salar	underyearlings; 1 - 1.5 g	underyearlings; 1 - 1.5 g	deriv GC-ECD	R	nw	6.3		10	15 d	0.0143	**690**	whole body ww	Cbiota/Cw	2	21	Carlberg et al., 1986
Trachurus novaezelandiae	caught in Sidney Harbour	ag	GC-MS	R	nw			21	7 d	0.1	95.87	muscles ww	(equilibrium) Cbiota/Cw or kinetic	2	5,21	Jennings et al, 1996
Not specified											269	whole body	Cbiota/Cw	4	6	Lu et al., 2000

Notes
1 Also described in EC, 2000
2 Analyses indicated that there was no significant volatilization or photodegradation of the chlorophenols after a 24h exposure period
3 Also described in EC, 2000 with BCF result of 14 - 125
4 Also described in EC, 2000 but with BCF result of 609-648
5 no bioconcentration detected in the liver
6 Review article; specific references per compound not specified
7 3 leaches per timepoint; steady state was reached within 5 days
8 3 leaches per timepoint; steady state was not reached during the experiment
9 only 1 leech used per experiment. May have been pre-exposed but probably not
10 Review
11 probably based on lipid weight; reported BCF does not equal reported concentrations; concentrations expressed as lipid and dry weight don't match reported percentages lipid and dry weight; field site is reported to be unpolluted;
12 field site is reported to be uncontaminated; exposure together with other phenolic compounds and sulfate soap to obtain an artificial effluent
13 Sand on the bottom (during the experiment 0.5% OM) ; plants present (1 g ww/L). Despite three times renewal of flow-through solution during the experiment, no water concentrations could be measured after 36 days. Biota concentrations still increased after this time.
14 BCF based on nominal concentrations and biota concentration at 45 days
15 BCF based on measured concentration at 36 days.
16 steady state was reached after 40 hours
17 Exposure duration is short, equilibrium might not be fully reached; aquaeous concentration presumably not measured

18 BCF based on total 14C amounts; nominal concentration was 0.05 mg/L; static system.
19 Not a really relevant life-stage for BCF determination; water concentration decreases to 20% of the initial concentration; various exposure times mentioned in the article.
20 BCF based on measured concentration at 21 days (maximum concentration in biota)
21 Number of 690 could not be reproduced from presented figure; Doubtful if equilibrium was achieved in the exposure time; Extrapolation of BCF estimated at different time intervals would probably lead to similar values

Appendix 2. Detailed aquatic toxicity data

Table A2.1 Acute toxicity of 2,3,4-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogenase activity	13	2	1	Liu et al., 1982
*Burkholderia RASC c*2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	1.93	2	2	Boyd et al., 2001
Pseudomonas fluorescens	soil bacteria, *lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	2.96	2	3	Boyd et al., 2001
Algae															
Chlorella vulgaris		N		rg	am				7 d	EC50	cell density	1.53	3	4	Yen et al., 2002
Pseudokirchneriella subcapitata	5E+04 cells/mL	N	S		am		21 ± 1		96 h	EC50	growth rate	2	2	5	Shigeoka et al., 1988
Cnidaria															
Hydra attennata	adult	N	R		am	7			44 h	LOEC	tulip stage	1	2	6	Mayura et al., 1991
Crustacea															
Daphnia magna	< 72 h old	N	S	> 95	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	2.24	2	7	Devillers et al., 1987; Devillers and Chambon, 1986a; Devillers and Chambon, 1986b
Pisces															
Danio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	1.92	2		Devillers and Chambon, 1986 b
Leuciscus idus melanotus			S			7-8	20	267	48 h	LC50	mortality	1.2	2	10	Rübelt et al., 1982
Poecilia reticulata		Y	S		tw	7.6 - 8		262	96 h	LC50	mortality	4.5	4	8	Dojlido, 1979
Tilapia zilli	2 - 6 cm	N	R	rg		6.6	25 ± 1	215		LC50	mortality	2.64	2	9	Yen et al., 2002

Notes
1 Species is relevant to the aquatic compartment
2 Test result is average of three replicates.
3 Test result is average of three replicates; soil bacteria which also occurs in freshwater .
4 Test duration > 96 h and unclear if cells are still in exponential growth phase.
5 Solvent DMSO is not toxic in solvent controls.
6 Criterion (tulip stage) considered relevant because it preceeds desintegration (mortality). Compound was purified prior to use.
7 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
8 Animals used were young adults just before they revealed sexual dimorphism; test substance unknown, only described as 'trichlorophenol'.
9 Test duration not reported, probably 96 hours.
10 According to standard German test methods (1974)

Table A2.2 Acute toxicity of 2,3,4-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am		15	21.9	30 min	EC50	bioluminescence	1.245825	2	1	Ribo and Kaiser, 1983
Vibrio fischeri		N	S		am	7	15	21.9	15 min	EC50	bioluminescence	4.126621	2	2	Svenson and Zhang, 1995
Vibrio fischeri		N	S		am	7.3	15	21.9	15 min	EC50	bioluminescence	4.442535	2	2	Svenson and Zhang, 1995
Crustacea															
Crangon septemspinosa	6.4 - 8.3 cm length, 2.4 - 4.5 g	Y	R		nw		10	30		LC50	mortality	2	3	3	McLeese et al., 1979
Pisces															
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	4.31	3	4	Smith et al., 1994

Notes
1 Microtox test. Data from 15 and 30 min-exposures are most accurate.
2 Microtox test.
3 Exposure time not fixed (time to lethality experiment). Unclear if LC50 is based on nominal or measured concentrations, but concentrations remained practically constant. 3 shrimp and 3 clams were exposed simultaneously. Number of test animals (3) too small
4 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L). Tightly fitted glass lid, aeration unclear

Table A2.3 Acute toxicity of 2,3,5-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Pure culture	grown in medium with phenol as pure carbon source; growth is not supported by chlorophenols	N	S		am	7.2	ca. 20			EC50	growth on phenol	90.3	3	1	Banerjee, 1987
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogenase activity	10.0	2	2	Liu et al., 1982
Burkholderia RASC c2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	1.26	2	3	Boyd et al., 2001
Pseudomonas fluorescens	soil bacteria, *lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	4.94	2	4	Boyd et al., 2001
Protozoa															
Tetrahymena pyriformis	2500 cells/mL, in log-phase	N	S	≥ 95	am	7.35	27 ± 1		48 h	EC50	population growth (density)	0.84	2	5	Bryant and Schultz, 1994
Cnidaria															
Hydra vulgaris	adult	N	R	purified	am	7			20 h	LOEC	tulip stage	1	2	6	Mayura et al., 1991
Crustacea															
Daphnia magna	< 72 h old	N	S	> 95	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	2.28	2	7	Devillers and Chambon, 1986a; Devillers and Chambon, 1986b; Devillers et al., 1987
Pisces															
Danio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	1.42	2		Devillers and Chambon, 1986a
Leuciscus idus melanotus			S			7-8	20	267	48 h	LC50	mortality	0.62	2	11	Rübelt et al., 1982
Poecilia reticulata		Y	S		tw	7.6 - 8		262	96 h	LC50	mortality	4.5	4	8	Dojlido, 1979
Poecilia reticulata	2 - 3 mo	N	R		am or rw	6.1	22 ± 1	25	7 or 14 d	LC50	mortality	0.88	2	9	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo	N	R		am or rw	7.3	22 ± 1	25	7 or 14 d	LC50	mortality	1.57	2	9	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo	N	R		am or rw	7.7 - 7.9	22 ± 1	25	7 or 14 d	LC50	mortality	4.74	2	9	Könemann and Musch, 1981
Salmo trutta	average 4.5 g	N		97			ca. 5		24 h	LC50	mortality	0.8	2		Hattula et al., 1981
Tilapia zilli	2 - 6 cm	N	R	rg		6.6	25 ± 1	215		LC50	mortality	1.29	2	10	Yen et al., 2002

Notes
1 Species unknown and endpoint irrelevant
2 Species is relevant to the aquatic compartment
3 Test result is average of three replicates.
4 Test result is average of three replicates; soil bacteria which also occurs in water.
5 Final DMSO concentration of 0.35 mL DMSO / 50 mL not toxic to Tetrahymena.
6 Tulip stage is followed by disintegration.
7 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
8 Animals used were young adults just before they revealed sexual dimorphism; test substance unknown, only described as 'trichlorophenol'.
9 Exposure duration (7 or 14 days) not clear; influence of pH on toxicity tested.
10 Test duration not reported, probably 96 hours.
11 According to standard German test methods (1974)

Table A2.4 Acute toxicity of 2,3,5-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am		15	21.9	30 min	EC50	bioluminescence	1.110343	2	1	Ribo and Kaiser, 1983
Vibrio fischeri		N	S		am	6.5 - 7.5	15		5 min	EC50	bioluminescence	0.67	2	2	Blum and Speece, 1991a and Blum and Speece, 1991b
Vibrio fischeri									30 min	EC50	bioluminescence	1.11032	4	3	Sixt and Altschuh, 1997
Pisces															
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	2.31	3	4	Smith et al., 1994

Notes
1 Microtox test. Data from 15 and 30 min-exposures are most accurate.
2 Microtox test.
3 Microtox test, from COMPUTOX database.
4 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L). Tightly fitted glass lid, aeration unclear.

rivm

Table A2.5 Acute toxicity of 2,3,6-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogen ase activity	190	2	1	Liu et al., 1982
*Burkholderia RASC c*2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	5.73	2	2	Boyd et al., 2001
Pseudomonas fluorescens	soil bacteria, *lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	18.2	2	3	Boyd et al., 2001
Cnidaria															
Hydra vulgaris	adult	N	R		am	7			68 h	LOEC	tulip stage	10.0	2	4	Mayura et al., 1991
Crustacea															
Astacus fluviatilis	males and females, captured in the field, 12 - 45 g	Y	R	> purum grade	dtw	7.5	13 ± 1	120	8 d	LC50	mortality	19.0	1		Kaila and Saarikoski., 1977
Astacus fluviatilis	males and females, captured in the field, 12 - 45 g	Y	R	> purum grade	dtw	6.5	13 ± 1	120	8 d	LC50	mortality	5.40	1		Kaila and Saarikoski., 1977
Daphnia magna	< 72 h old	N	S	> 95	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	7.39	2	5	Devillers and Chambon, 1986a Devillers and Chambon, 1986b Devillers et al., 1987
Pisces															
Brachydanio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	7.42	2		Devillers and Chambon, 1986 b
Leuciscus idus melanotus			S			7-8	20	267	48 h	LC50	mortality	2.9	2	10	Rübelt et al., 1982
Oncorhynchus mykiss	4.6 - 6.4 cm, 1.2 - 3.8 g	Y	CF	≥ 98	tw	7.6 - 8.2	14.1 - 16.5		96 h	LC50	mortality	1.90	2	6	Hodson et al., 1984
Poecilia reticulata		Y	S		tw	7.6 – 8		262	96 h	LC50	mortality	4.50	4	7	Dojlido, 1979
Poecilia reticulata	2 - 3 mo		R		am or rw	6.1	22 ± 1	25	7 or 14 d	LC50	mortality	0.95	2	8	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo		R		am or rw	7.3	22 ± 1	25	7 or 14 d	LC50	mortality	5.08	2	8	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo		R		am or rw	7.7 - 7.9	22 ± 1	25	7 or 14 d	LC50	mortality	13.3	2	8	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo old males			rg	tw	7.7			24 h	LC50	mortality	10.5	4	9	Benoit-Guyod et al., 1984

Notes
1 Species is relevant to the aquatic compartment.
2 Test result is average of three replicates.
3 Test result is average of three replicates; soil bacteria which also occurs in freshwater.
4 Criterion (tulip stage) considered relevant because it preceeds desintegration (mortality). Compound was purified prior to use.
5 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
6 Test result is mean of 3 bioassays. Oxygen concentration may have been low (range of all experiments: 5.6 - 9.4 mg/L O_2 at 14.1 - 16.5 °C); results based on mean measured concentrations.
7 Animals used were young adults just before they revealed sexual dimorphism; test substance unknown, only described as 'trichlorophenol'.
8 Exposure duration (7 or 14 days) not clear; influence of pH on toxicity tested.
9 Unit of LC50 not reported; calculated from log 1/LC50 assuming it is given in mol/L.
10 According to standard German test methods (1974)

Table A2.6 Acute toxicity of 2,3,6-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am		15	21.9	30 min	EC50	bioluminescence	12.7	2	1	Ribo and Kaiser, 1983
Vibrio fischeri		N	S		am	6.5 - 7.5	15		5 min	EC50	bioluminescence	2.1	2	1	Blum and Speece, 1991a Blum and Speece, 1991b
Crustacea															
Crangon septemspinosa	6.4 - 8.3 cm length, 2.4 - 4.5 g	Y	R		nw		10	30	96 h	LC50	mortality	2.70	3	2	McLeese et al., 1979
Pisces															
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	4.40	3	3	Smith et al., 1994
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	5.67	3	3	Smith et al., 1994
Solea solea	collected in the field, 45 ± 2.5	Y	R	≥ 98		8 ± 0.1	6	22	96 h	LC50	mortality	2.13	3	4	Smith et al., 1994

Notes
1 Microtox test.
2 Exposure time not fixed (time to lethality experiment). Unclear if LC50 is based on nominal or measured concentrations, but concentrations remained practically constant. 3 shrimp and 3 clams were exposed simultaneously.
3 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L). Tightly fitted glass lid, aeration unclear.
4 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (27 g/L instead of 1 g/L).

Table A2.7 Acute toxicity of 2,4,5-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Pure culture		N	S		am	7.2	ca. 20		Exp. Gr. phase	EC50	growth on phenol	56.9	3	1	Banerjee, 1987
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogenase activity	12.0	2	2	Liu et al., 1982
Bacillus subtilis						7.2				EC50	spore germination	25.3	4	3	Yasuda et al., 1982
Burkholderia RASC c2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	1.20	2	4	Boyd et al., 2001
Escherichia coli	10E4 cells/mL, in log phase	N	S	≥ 98	am		37			LOEC	cell density	8.89	4	5,6	Nendza and Seydel, 1990
Escherichia coli	10E4 cells/mL	N	S		am		37			EC50	growth rate	8.29	4	6	Nendza and Seydel, 1988a Nendza and Seydel, 1988b Nendza and Seydel, 1990
Mycobacterium smegmatis	10E4 cells/mL, in log phase	N	S	≥ 98	am		37			LOEC	cell density	8.89	4	5,6	Nendza and Seydel, 1990
Pseudomonas										NOEC	growth	≥ 20	4		Rübelt, 1994
Pseudomonas fluorescens	soil bacteria, *lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	11.3	2	7	Boyd et al., 2001
Algae															
Chlorella vulgaris		N		rg	am				7 d	EC50	cell density	1.23	3	8	Yen et al., 2002
Phormidium									24 h	EC100		0.10	3	9	German Chemical Society, 1994
Protozoa															
Tetrahymena pyriformis		Y		≥ 95					48 h	EC50	population growth (density)	1.58	2	10	Schultz et al., 1996
Tetrahymena pyriformis	strain GL-C	N	S	> 95	am	7.35	27 ± 1	75	40 h	EC50	population growth (cell density)	1.57	4*	11	Schultz, 1999
Tetrahymena pyriformis	ca. 36000 cells/mL, in log phase	N	S	≥ 95	am	7.35	27 ± 1		48 h	EC50	population growth (density)	1.57	4*	12	Schultz et al., 1990
Tetrahymena pyriformis	2500 cells/mL, in log-phase	N	S	≥ 95	am	7.35	27 ± 1		48 h	EC50	population growth (density)	1.57	2	13	Bryant and Schultz, 1994
Tetrahymena pyriformis		N	S	ag	am		30		24 h	EC50	cell number	0.68	2	14	Yoshioka et al., 1985
Macrophyta															
Lemna gibba	5 - 7 3-frond colonies (15 - 21 fronds total)	N							7 d	EC50	vegetative frond reproduction	0.41	3	15	Sharma et al., 1997
Lemna minor		Y		>98	am	6.8 - 7.2	17			EC50	yield (dry weight)	0.73	2	16	Neilson et al., 1990
Lemna minor		Y		>98	am	5.8	17			EC50	yield (dry weight)	0.56	2	16	Neilson et al., 1990
Lemna minor		Y		>98	am	6.8	17			EC50	yield (dry weight)	0.86	2	16	Neilson et al., 1990
Lemna minor		Y		>98	am	7.5	17			EC50	yield (dry weight)	2.2	2	16	Neilson et al., 1990
Lemna minor		N	S			5.1	25 ± 1		48 h	LC50	mortality (chlorosis)	1.6	3	17	Blackman et al., 1955
Fungi															
Pichia	fermentative strain from dinitrification stage of STP	N	S		am	7	22 ± 2		12 h	EC50	growth (turbidity)	4.30	2	18	Kwasniewska and Kaiser, 1983
Rhodotorula rubra	oxidative strain from shore of Lake Ontario	N	S		am	7	22 ± 2		12 h	EC50	growth (turbidity)	2.0	2	18	Kwasniewska and Kaiser, 1983
Saccaromyces	mutant capable of thymidine assimilation; 1.3E+07 cells/mL	N	S		am		30		7 h	EC50	growth (dry weight)	5.92	2	19	Guerra and Lochmann, 1988
Cnidaria															
Hydra vulgaris	adult	N	R	purified	am	7			28 h	LOEC	tulip stage	1.00	2	20	Mayura et al., 1991
Mollusca															

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Lymnaeidae									24 h	LC100	mortality	10	4		German Chemical Society, 1994
Annelida															
Lumbriculus variegatus	7 ± 3 mg	Y	S	> 99	am	6.5 ± 0.1	20 ± 1	50	48 h	LC50	mortality	0.9	2	21	Kukkonen, 2002
Crustacea															
Ceriodaphnia dubia		Y	R		nw	7.6 - 7.9	25	44	48 h	LC50	mortality	1.74	2	22	Spehar, 1986
Ceriodaphnia dubia	< 24 h old	N	S				23 ± 1		48 h	EC50	immobility	1.21	2		Westbury, 1998
Daphnia magna	< 24 h old		S		am				24 h	LC50	mortality	4.79	2	24	LeBlanc et al., 1988
Daphnia magna	< 24 h old	N	S	≥ 80%	rw	7.4 - 9.4	22 ± 1	173 ± 13	48 h	LC50	mortality	2.70	2	23	LeBlanc, 1984
Daphnia magna	< 24 h old	N	S	≥ 80%	rw	7.4 - 9.4	22 ± 1	173 ± 13	48 h	NOEC	mortality	0.78	2	23	LeBlanc, 1984
Daphnia magna		Y				7.9 - 8.1	20		48 h	LC50	mortality	1.60	2	25	Neilson et al., 1990
Daphnia magna		Y				6.2	20		48 h	LC50	mortality	0.29	2	25	Neilson et al., 1990
Daphnia magna		Y				7.2	20		48 h	LC50	mortality	0.69	2	25	Neilson et al., 1990
Daphnia magna		Y				8.2	20		48 h	LC50	mortality	2.60	2	25	Neilson et al., 1990
Daphnia magna	6 - 24 h old	N	S		am	8.0 ± 0.2	20	240	48 h	EC50	immobility	0.90	2	26	Kühn et al., 1989a
Daphnia magna		N	S		Am		20	250	24 h	EC50	Immobility	1.20	2	27	Knie et al., 1983
Daphnia magna	≤ 24 h old		S		am	8.0 ± 0.2	20	250	24 h	EC50	immobility	1.30	2		Bringmann and Kühn, 1982
Daphnia magna	< 24 h old	N	S	> 98			20 ± 1		48 h	EC50	immobility	0.97	2	28	Steinberg et al., 1992
Daphnia magna	< 24 h old	N	S	> 98			20 ± 1		48 h	EC50	immobility	1.01	3	29	Steinberg et al., 1992
Daphnia magna	< 24 h old	N	S	> 98			20 ± 1		48 h	EC50	immobility	1.10	2	30	Steinberg et al., 1992
Daphnia magna	< 24 h old	N	S	> 98			20 ± 1		48 h	EC50	immobility	1.04	3	31	Steinberg et al., 1992
Daphnia magna	< 72 h old	N	S	> 95%	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	2.08	2	32	Devillers and Chambon, 1986a Devillers and Chambon, 1986b Devillers et al., 1987
Daphnia magna	<24h	N	S		rw	8	25	150	48 h	LC50	mortality	2.08	2		Kim et al., 2006
Pisces															
Carassius auratus	1.0 ± 0.1 g		S	± 100	tw	7.0 ± 0.1	27 - 28		5 h	LC50	mortality	0.93	3	50	Kishino and Kobayshi, 1996a
Carassius auratus	1.0 ± 0.1 g	N	S	± 100	tw	7.0 ± 0.1	27 - 28		2.5 h	LC50	mortality	1.00	3	50	Kishino and Kobayshi, 1996b
Carassius auratus	2.2 ± 0.2 g		S	± 100	tw	6	20 - 21		5 h	LC50	mortality	*0.7 - 1*	3	49	Kishino and Kobayashi, 1995
Carassius auratus	2.2 ± 0.2 g		S	± 100	tw	8	20 - 21		5 h	LC50	mortality	*1.5 - 3*	3	49	Kishino and Kobayashi, 1995
Carassius auratus	2.2 ± 0.2 g		S	± 100	tw	10	20 - 21		5 h	LC50	mortality	*> 50*	3	49	Kishino and Kobayashi, 1995
Carassius auratus	2 g		R				20		24 h	LC50	mortality	1.70	2		Kobayashi et al., 1979
Carassius auratus									24 h	LC50	mortality	1.70	4		Verschueren, 1983
Carassius auratus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	39	Wood, 1953
Carassius auratus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	39	Hollis and Lennon, 1954
Danio rerio	adults	Y				7.2 - 7.5	24		96 h	LC50	mortality	0.53	2		Neilson et al., 1990
Danio rerio	larvae	Y	R	> 98		7.2 - 7.5	24		96 h	LC50	mortality	0.40	2		Neilson et al., 1990
Danio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	1.33	2		Devillers and Chambon, 1986a
Lepomis macrochirus	0.32 - 1.2 g ww	N	S	≥ 80%	am	6.5 - 7.9	21 - 23	32 - 48	96 h	LC50	mortality	0.45	2	48	Buccafusco et al., 1981
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		2 h	LOEC	mortality/ obvious distress	5.00	3	35	Applegate et al., 1957
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		2 h	LOEC	mortality/ obvious distress	5.00	3	35	Applegate et al., 1957
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	35	Applegate et al., 1957
Lepomis macrochirus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	39	Wood, 1953
Lepomis macrochirus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	39	Hollis and Lennon, 1954
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	35	Applegate et al., 1957

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Leuciscus idus							20	267	48 h	LC50	mortality	1.00	2		Dietz and Traud, 1978
Leuciscus idus		N					10 - 20			LC50	mortality	1.00	4*	33	Knie et al., 1983
Leuciscus idus melanotus			S			7-8	20	267	48 h	LC50	mortality	0.40	2	51	Rubelt et al., 1994
Oncorhynchus kisutch						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	34	Macphee et al., 1969
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	35	Applegate et al., 1957
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		2 h	LOEC	mortality/ obvious distress	5.00	3	35	Applegate et al., 1957
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	35	Applegate et al., 1957
Oncorhynchus mykiss									48 h	LC50	mortality	1.00	4		Anonymous, 1985
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		0.5 h	LOEC	mortality/ obvious distress	5.00	3	35	Applegate et al., 1957
Oncorhynchus mykiss		Y	F		nw	7.75	9.8	46	96 h	LC50	mortality	0.26	2	36	Spehar, 1986
Oncorhynchus tshawytscha						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	3	34	Lipnick et al., 1985
Oryzias latipes			R		tw	7.2	20 ± 1	40	48 h	LC50	mortality	13.00	2	37	Yoshioka and Ose, 1993
Oryzias latipes			R						48 h	LC50	mortality	12.30	4	38	Yoshioka et al., 1986a
Perca flavescens	fingerlings < 10.2 cm					7	12.8	300	1 h	LOEC	mortality	5.00	3	39	Wood, 1953
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		3 h	LOEC	mortality/ obvious distress	5.00	3	40	Applegate et al., 1957
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		3 h	LOEC	mortality/ obvious distress	5.00	3	40	Applegate et al., 1957
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	40	Applegate et al., 1957
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality/ obvious distress	≥ 1	3	40	Applegate et al., 1957
Pimephales promelas									96 h	LC50	mortality	2.73	4	41	Eldred, et al, 1999
Pimephales promelas	larvae, 0.509 mg	Y	R	99.5	nw			44 - 49	7 d	NOEC	growth (body weight) survival	0.36	2		Norberg-King, 1989.
Pimephales promelas	larvae, 0.509 mg	Y	R	99.5	nw			44 - 49	96 h	LC50	mortality	0.90	2		Norberg-King, 1989
Pimephales promelas	larvae, 0.509 mg	Y	R	99.5	nw			44 - 49	7 d	LC50	mortality	0.74	2		Norberg-King, 1989
Pimephales promelas		Y	F		nw	7.7-7.8	25	46	96 h	LC50	mortality	1.27	2	36	Spehar, 1986
Poecilia reticulata	40 - 60 mg	Y	R	≥ ag	Dw	6 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	0.99	2	42	Saarikoski and Viluksela, 1981
Poecilia reticulata	40 - 60 mg	Y)	R	≥ ag	Dw	7 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	1.24	2	42	Saarikoski and Viluksela, 1981
Poecilia reticulata	40 - 60 mg	Y	R	≥ ag	Dw	8 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	3.06	2	42	Saarikoski and Viluksela, 1981
Poecilia reticulata	40 - 60 mg		R			6	26 ± 1		96 h	LC50	mortality	0.99	4*		Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg		R			7	26 ± 1		96 h	LC50	mortality	1.25	4*		Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg		R			8	26 ± 1		96 h	LC50	mortality	3.06	4*		Saarikoski and Viluksela, 1982
Poecilia reticulata	2 - 3 mo old males			rg	tw	7.7 ± 0.1			24 h	LC50	mortality	0.53	4	43	Benoit-Guyod et al., 1984
Poecilia reticulata	40 - 60 mg	Y	R		dtw	7	25-27		96 h	LC50	mortality	1.20	2	44	Salkinoja-Salonen et al., 1981
Ptychochelilus oregonensis						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	45	Lipnick et al., 1985
Salmo trutta	average 4.5 g						ca. 5		24 h	LC50	mortality	0.90	2		Hattula et al., 1981
Salmo trutta	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	39	Wood, 1953
Salmo trutta	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	1.00	3	46	Hollis and Lennon, 1954
Tilapia zilli	2 - 6 cm	N	R	rg		6.6	25 ± 1	215		LC50	mortality	3.03	2	47	Yen et al., 2002

Notes

1 Species unknown; endpoint not relevant; grown in medium with phenol as pure carbon source; growth is not supported by chlorophenols.
2 Species is relevant to the aquatic compartment.
3 Mean of three determinations; test duration not clear.
4 Test result is average of three replicates.
5 Reported as Minimal Inhibition Concentration (MIC).
6 original reference unclear; test duration not reported.
7 Test result is average of three replicates; soil bacteria which also occurs in water.
8 Test duration > 96 h and unclear if cells are still in exponential growth phase.
9 Test endpoint reported as "complete inhibition". Unclear which test criterion is used.
10 ≤ 0.7% DMSO. Unclear if the EC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 80% of nominal in an abiotic control; same as Bryant and Schultz.
11 8 - 9 cell cycles; Same as Bryant and Schultz.
12 Same as Bryant and Schultz.
13 Final DMSO concentration of 0.35 mL DMSO / 50 mL not toxic to Tetrahymena.
14 Sealed for volatile compounds; < 5000 mg/L DMSO (non-toxic) for slightly soluble substances.
15 Test substances remained unchanged in abiotic control, but duckweed was able to metabolise test substance (95% within the first 4 d of growth). Study deemed unreliable because of possible metabolic transformation
16 Exposure duration not reported, but in accordance with U.S. EPA (1985). Results based on measured concentrations.
17 Fronds were considered to be dead when they were colorless over more than half the surface of the bath. Study deemed unreliable because of possible metabolic transformation.
18 Turbidity test.
19 EC50 calculated by fitting a logistic dose response model through data presented by author.
20 Criterion (tulip stage) considered relevant because it preceeds desintegration (mortality).
21 Test result is based on measured initial concentrations.
22 Results based on measured concentrations; According to methods described by Mount and Norbery (1984).
23 In accordance with U.S. EPA (1975).
24 In accordance with U.S. EPA (1975). Ethanol as solvent (< 0.05%). LC50 calculated by fitting a logistic dose response model through data presented by author.
25 In accordance with ISO (1985).
26 In accordance with DIN 38412, Part II 1982.
27 In accordance with DIN 38412 Teil 11.
28 No dissolved humic material (DHM); 2 h pretest contact time of DHM and test substance.
29 5 ppm dissolved humic material; 2 h pretest contact time of DHM and test substance.
30 No dissolved humic material (DHM); 60 h pretest contact time of DHM and test substance.
31 5 ppm dissolved humic material (DHM); 60 h pretest contact time of DHM and test substance.
32 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
33 In accordance with DIN 38412 Teil 15.
34 Endpoint unclear. Reported as time to effect.
35 Only two fish were tested. Reported as time to effect. Up to three fish species were tested simultanuously.
36 Results based on measured concentrations. According to ASTM test protocols.
37 In accordance with OECD 203.
38 In accordance with OECD 203 (1982); unit LC50 not reported.
39 Reported as time to effect. Only two fish tested.
40 Only two fish were tested. Reported as time to effect. Up to three fish species were tested simultanuously. Sea Lamprey occur in the american great lakes (freshwater).
41 Data from COMPUTOX database.
42 Preliminary test showed that in 12 hours, less than 5% of the compound disappeared.
43 Unit of LC50 not reported; calculated from log 1/LC50, assuming LC50 is given in mol/L.
44 Unclear if results are based on measured or nominal concentrations; measured concentrations close to nominal concentrations.
45 Reported as time to effect.
46 Reported as time to effect. Only two fish tested.
47 Test duration not reported, probably 96 hours.
48 Dissolved oxygen concentrations too low (range: 9.7 at start - 0.3 mg/L after 96 h) for a number of the compounds tested). Not clear if this was also the case for this compound. In accordance with U.S. EPA 1975.
49 No control group included. A 5-h exposure period was chosen, because within this period, no detoxification of the test substance occurred. LC50 are only indicative values, because not all concentrations were observed until 5 hours.
50 No control group included.
51 According to standard German test methods (1974)

Table A2.8 Acute toxicity of 2,4,5-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am		15	21.9	15 min	EC50	bioluminescence	1.217467	2	1	Ribo and Kaiser, 1983
Vibrio fischeri									3 min	EC50	bioluminescence	20.62	2	1	Lee et al., 1999
Vibrio fischeri									10 min	EC50	bioluminescence	12.66	2	2	Lee et al., 1999
Vibrio fischeri									20 min	EC50	bioluminescence	7.77	2	2	Lee et al., 1999
Vibrio fischeri		N			am				5 min	EC50	bioluminescence	1.184676	2	6	Ribo and Rogers, 1990
Vibrio fischeri		N			am				15 min	EC50	bioluminescence	1.184676	2	6	Ribo and Rogers, 1990
Vibrio fischeri	ahs98 (antibiotic hypersensitive mutant of strain NRRL B-11177 (1.0E+06 cells/mL)				am		20	21.9	30 min	EC50	bioluminescence	1.405233	3	3	Wagner et al., 1989
Vibrio fischeri		Y				6.2	15		15 min	EC50	bioluminescence	0.6	2	4	Neilson et al., 1990
Vibrio fischeri		Y				7.2	15		15 min	EC50	bioluminescence	1.2	2	4	Neilson et al., 1990
Vibrio fischeri		Y				8.2	15		15 min	EC50	bioluminescence	9.5	2	4	Neilson et al., 1990
Vibrio fischeri		N	S				15		5 min	EC50	bioluminescence	2.042	2	4	Westbury, 1998
Vibrio fischeri	strain NRRL-B-11177	Y	S	99	am		15 ± 0.2		30 min	EC50	bioluminescence	1.021833	2	5	Froehner et al., 2002
Vibrio fischeri		N	S		am		15 ± 0.1	21.9	5 min	EC50	bioluminescence	1.8	2	4	Somasundaram et al., 1990
Algae															
Skeletonema costatum									96 h	EC50	cell number	0.96	4		US EPA, 1979
Mollusca															
Mya arenaria	ca. 5 cm length, 20 g	Y	R		nw		10	30	96 h	LC50	mortality	2.4	3	7	McLeese et al., 1979.
Annelida															
Platynereis dumerilii	newly fertilised embryos (< 6 h post-fertilization)	N	S	> 99	nw	8.01 - 8.13	19.2 - 20.3	34.9	48 h	EC50	embryo development	2.55	2	8	Palau and Hutchinson, 1998
Platynereis dumerilii	7-d old larvae	N	S	> 99	nw	8.01 - 8.13	19.2 - 20.3	34.9	96 h	LC50	mortality	4.24	2		Palau and Hutchinson, 1998
Crustacea															
Mysidopsis bahia	juvenile								96 h	LC50	mortality	3.751474	4	9	LeBlanc et al., 1988
Mysidopsis bahia									96 h	LC50	mortality	3.83	4		German Chemical Society, 1994
Palaemonetes pugio	intermoulting adults, field collected; 25 mm	N	R	94		7.6 - 7.7	20	10	96 h	LC50	mortality	1.1	2	10	Rao et al., 1981
Palaemonetes pugio	moulting adults, field collected; 25 mm	N	R	94		7.6 - 7.7	20	10	96 h	LC50	mortality	0.64	2	11	Rao et al., 1981
Tisbe battagliai	6 d old copepodid stages		S	≥ 98	nw	8.0 ± 0.1	20	30	24 h	LC50	mortality	2.442407	2		Smith et al., 1994
Pisces															
Cyprinodon variegatus	juveniles, 14 - 28 d posthatch, 8 - 15 mm		S	≥ 80	nw		25 - 31	10 - 31	96 h	LC50	mortality	1.7	2	12	Heitmuller et al., 1981
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	4.01	3	13	Smith et al., 1994

Notes
1 Microtox test.
2 Microtox test. Article in chinese language. Data from 15 and 30 min-exposures are most accurate.
3 EC50 determined from figure using TechDig. Mutagenesis induced by chemical to obtain more sensitive mutant. Unit of EC50 is not reported.
4 Microtox test.
5 EC50 calculated by fitting a logistic dose response model through data presented by author.
6 Microtox test. Tested with highest purity commercially available.
7 Exposure time not fixed (time to lethality experiment). Unclear if LC50 is based on nominal or measured concentrations, but concentrations remained practically constant. 3 shrimp and 3 clams were exposed simultaneously. Number of test animals too small.
8 Percentage of embryos developing normally was calculated in accordance with ASTM 1989.
9 Original reference difficult to obtain.
10 Intermoult.
11 Moulting.
12 In accordance with EPA-660/3-75-009.
13 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L). Tightly fitted glass lid, aeration unclear.

Table A2.9 Chronic toxicity of 2,4,5-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Chlorella pyrenoidosa										LOEC		1.5	4	2	Jones, 1971 In: German Chemical Society, 1994
Chlorella pyrenoidosa		N	S		am	7	22		72h	NOEC	chlorophyll/ oxygen production	1	3	3	Huang and Gloyna, 1968
Nitzschia sp.		Y		>98	am	6.8 - 7.2	17			NOEC	growth rate	0.1	4	2	Neilson et al., 1990
Scenedesmus sp.		Y		>98	am	6.8 - 7.2	17			NOEC	growth rate	0.24	2	5	Neilson et al., 1990
Scenedesmus subspicatus		N	S		am	7	27	550	8 d	LOEC	growth	1.11	2	6	Schmidt and Schnabl, 1988
Scenedesmus subspicatus					am	7	27	550	8 d	LOEC	Fluores-cence	0.49	2	7	Schmidt and Schnabl, 1988
Cyanobacteria															
Anabaena sp.		Y		>98	am	6.8 - 7.2	17			NOEC	growth rate	0.115	2	1	Neilson et al., 1990
Macrophyta															
Lemna gibba	5 - 7 3-frond colonies (15 - 21 fronds total)	N							7 d	EC10	vegetative frond reproduction	0.12	3	8	Sharma et al., 1997
Crustacea															
Ceriodaphnia dubia		Y	R		nw	7.6 - 7.9	25	44	7 d	NOEC	number of offspring	0.375	9	1	Spehar, 1986
Ceriodaphnia dubia		Y	R		nw	7.6 - 7.9	25	44	7 d	NOEC	survival	0.746	9	1	Spehar, 1986
Pisces															
Danio rerio		Y				6.2				LOEC		0.15	4	10	Neilson et al., 1990
Danio rerio		Y				7.2				LOEC		0.15	4	10	Neilson et al., 1990
Danio rerio		Y				8.2				LOEC		0.4	4	10	Neilson et al., 1990
Oncorhynchus mykiss	larvae	Y	F		nw (filtered)	7.75	9.6	45	90d	NOEC	survival	0.108	1	11	Spehar, 1986
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	growth (ww)	0.297	1	12	Arthur and Dixon, 1994
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	survival	≥ 0.863	1	12	Arthur and Dixon, 1994
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	growth (ww)	0.536	1	13	Arthur and Dixon, 1994
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	survival	≥ 0.863	1	13	Arthur and Dixon, 1994
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	growth (ww)	0.536	1	14	Arthur and Dixon, 1994
Pimephales promelas	< 1 d old	Y	CF	> 98	nw	7.8 ± 0.1	23 - 25	392	28 d	NOEC	survival	≥ 0.863	1	14	Arthur and Dixon, 1994
Pimephales promelas	larvae	Y	F		nw (filtered)	7.7-7.9	25	45-46	32 d	NOEC	survival	0.16	1	11	Spehar, 1986

Notes

1 Calculated from EC20: NOEC = 0.23 / 2. Exposure duration not reported, but in accordance with OECD (1984).
2 Toxic at reported value; assumed that the LOEC is ment.
3 Cell densitiy too high.
4 Calculated from EC20: NOEC = 0.2 / 2. Exposure duration not reported, but in accordance with OECD (1984).
5 Calculated from EC20: NOEC = 0.48 / 2. Exposure duration not reported, but in accordance with OECD (1984).
6 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control and thus an unknown % effect.
7 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control and thus an unknown % effect. Relevant endpoint since chlorophenols uncouple electron transport.
8 Test substances remained unchanged in abiotic control, but duckweed was able to metabolise test substance (95% within the first 4 d of growth). Thus, test result deemed unreliable.
9 Results based on measured concentrations, According to methods described by Mount and Norbery (1984).
10 modified ELS test? Not clear in text.
11 Results based on measured concentrations; According to ASTM test protocols.
12 Effect of rearing density: 1 fish/L. In accordance with EPA/600/4-89/001.
13 Effect of rearing density: 5 fish/L. In accordance with EPA/600/4-89/001.
14 Effect of rearing density: 10 fish/L. In accordance with EPA/600/4-89/001.

rivm

Table A2.10 Chronic toxicity of 2,4,5-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri	strain NRRL-B-11177	Y	S	99	am		15 ± 0.2		24 h	EC10	Biolumi-nescence	0.44	2	1	Froehner et al., 2002
Algae															Lee et al., 1999
Champia parvula	tetrasporophytes	N	R		am		22 - 24	30	11 - 14 d	NOEC	vegetative growth (dw)	0.232	2		Thursby et al., 1985
Champia parvula	females	N	R		am		22 - 24	30	11 - 14 d	NOEC	vegetative growth (dw)	0.999	2		Thursby et al., 1985
Champia parvula		N	R		am		22 - 24	30	11 - 14 d	NOEC	number of reproductive structures/mg dw	0.232	2		Thursby et al., 1985
Champia parvula		N	R		am		22 - 24	30	11 - 14 d	NOEC	reproduction (no of asexual spores)	< 0.552	2	2	Thursby et al., 1985
Champia parvula		N	R		am		22 - 24	30	11 - 14 d	NOEC	Reproduc-tion (absence of sexual reproduction)	4.62	2		Thursby et al., 1985
Champia parvula		N	R		am		22 - 24	30	11 - 14 d	NOEC	Reproduc-tion (absence of asexual reproduction)	7.536	2		Thursby et al., 1985

Notes
1 EC10 calculated by fitting a logistic dose response model through data presented by author.
2 NOEC was calculated from MATC as follows: MATC/SQRT(2).

Table A2.11 Acute toxicity of 2,4,6-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogenase activity	240.00	2	1	Liu et al., 1982
Bacillus subtilis						7.2				EC50	spore germination	25.67	4	2	Yasuda et al., 1982
Burkholderia RASC c2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	14.81	2	3	Boyd et al., 2001
Escherichia coli	HB101 pUCD607	N	S	> 99.5	dw	5.5			20 min	EC50	bioluminescence	27.64	2		Tiensing et al., 2002
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	EC50	specific growth rate	31.59	2	4	Cenci et al., 1987
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	EC50	dehydrogenase activity	49.36	2	4	Cenci et al., 1987
Escherichia coli	10E4 cells/mL, in log phase	N	S	tg	am		37			LOEC	cell density	71.08	4	5	Nendza and Seydel, 1990
Escherichia coli	10E4 cells/mL	N	S		am		37			EC50	growth rate	37.51	4	6	Nendza and Seydel, 1988a Nendza and Seydel, 1988b Nendza and Seydel, 1990
Mycobacterium smegmatis	10E4 cells/mL, in log phase	N	S	tg	am		37			LOEC	cell density	25.67	4	5	Nendza and Seydel, 1990
Pseudomonas fluorescens	10586r pUCD607	N	S	> 99.5	dw	5.5			20 min	EC50	bioluminescence	11.85	2		Tiensing et al., 2002
Pseudomonas fluorescens	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	5.13	2	3	Boyd et al., 2001
Salmonella typhimurium	TA98				am	6.6	37		30 min	EC50	specific growth rate	47.39	3	8	Pill et al., 1991
Algae															
Chlorella vulgaris		N		rg	am				7 d	EC50	cell density	3.20	3	9	Yen et al., 2002
Chlorella vulgaris	5E+04 cells/mL	N	S		am		21 ± 1		96 h	EC50	growth rate	10.00	2	10	Shigeoka et al., 1988
Chlorella pyrenoidosa	1e+5 cells/ml	N	S		am		18		12 d	EC100	number of cells	1.00	3	11	Rowe et al., 1982
Pseudokirchneriella subcapitata	5E+04 cells/mL	N	S		am		21 ± 1		96 h	EC50	growth rate	3.50	2	10	Shigeoka et al., 1988
Scenedesmus subspicatus	ca. 10^4 cells/mL	N	S	98	am	7	22 ± 2	550	96 h	EC50	biomass (AUC)	5.60	2	12	Geyer et al., 1985
Protozoa															
Spirostomum teres	from log growing cultures		S	> 98	dw		25		24 h	LC50	mortality	2.00	2		Twagilimana et al., 1998
Tetrahymena pyriformis	strain GL-C	N	S	> 95	am	7.35	27 ± 1	75	40 h	EC50	population growth (cell density)	7.68	2	13	Schultz et al., 1986 Schultz, 1997 Schultz, 1999
Tetrahymena pyriformis	strain GL, 10^4 cells/mL, exp. growth phase	N	S	≥ 98	am		28		9 h	EC50	population growth (cell density)	3.00	2	15	Bogaerts et al., 1998
Tetrahymena pyriformis	ca. 36000 cells/mL, in log phase	N	S	≥ 95	am	7.35	27 ± 1		48 h	EC50	population growth (density)	3.94	2	13	Schultz et al., 1990
Tetrahymena pyriformis			S						60 h	EC50	population growth (density)	3.99	4*	13	Schultz and Riggin, 1985
Tetrahymena pyriformis		N	S	ag	am		30		24 h	EC50	population growth	3.10	2	16	Yoshioka et al., 1985
Macrophyta															
Lemna minor		Y		>98	am	6.8 - 7.2	17			EC50	yield (dry weight)	0.50	2	17,43	Neilson et al., 1990
Lemna minor		N	S			5.1	25 ± 1		48 h	LC50	mortality (chlorosis)	5.60	3	18	Blackman, et al., 1955
Fungi															
Saccharomyces	mutant capable of thymidine assimilation; 1.3E+07 cells/mL	N	S		am		30		7 h	EC50	growth (dry weight)	11.22	2	7	Guerra and Lochmann, 1988
Cnidaria															
Hydra vulgaris	adult									LOEC	maternal toxicity	8.00	4	19	Fu et al., 1990

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Hydra vulgaris	adult	N	R	purified	am	7			28 h	LOEC	tulip stage	10.00	2	20	Mayura et al., 1991
Platyhelmintes															
Dugesia japonica	collected in the field, ca. 2 cm-long animals cut into body parts	N	R	ag	am		20 ± 1		7 d	EC50	head regeneration	7.08	2	21	Yoshioka et al., 1986a
Dugesia japonica	collected in the field, ca. 2 cm-long animals cut into body parts	N	R	ag	am		20 ± 1		7 d	LC50	mortality	8.91	2	21	Yoshioka et al., 1986a
Mollusca															
Aplexa hypnorum	adults	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	96 h	LC50	mortality	5.50	2	22	Holcombe et al., 1987
Annelida															
Lumbriculus variegatus	7 ± 3 mg	Y	S	> 98	am	6.5 ± 0.1	20 ± 1	50	48 h	LC50	mortality	1.36	2	23	Kukkonen, 2002
Crustacea															
Ceriodaphnia dubia	< 24 h old						22		48 h	EC50	immobility	4.00	4*	24	Bitton et al., 1995
Ceriodaphnia dubia	< 24 h old	N			rw		22		48 h	EC50	immobility	4.00	2	25	Bitton et al., 1996
Ceriodaphnia dubia	< 24 h old	N	S				23 ± 1		48 h	EC50	immobility	1.65	2		Mulhall, 1997 In: Warne and Westbury, 1999
Ceriodaphnia dubia	< 24 h old	Y	S				23 ± 1		48 h	EC50	immobility	1.74	2		Westbury, 1998
Daphnia carinata	< 24 h old	N	S				20 ± 1		48 h	EC50	immobility	0.56	2		Azim, 1998 In: Warne and Westbury, 1999
Daphnia magna		Y		99.3	rw	9.5	20 ± 2	250 ± 25	24 h	EC50	immobility	14.60	3	26	Tissot et al., 1985
Daphnia magna	< 24 h old	N	S	≥ 80	rw	7.4 - 9.4	22 ± 1	173 ± 13	48 h	LC50	mortality	6.00	2	27	LeBlanc, 1984
Daphnia magna	< 24 h old	N	S	≥ 80	rw	7.4 - 9.4	22 ± 1	173 ± 13	48 h	NOEC	mortality	< 0.41	2	27	LeBlanc, 1984
Daphnia magna		Y				7.9 - 8.1	20		48 h	LC50	mortality	4.50	2	28,43	Neilson et al., 1990
Daphnia magna	6 - 24 h old	N	S		am	8.0 ± 0.2	20	240	48 h	EC50	immobilisation	2.20	2	29	Kühn et al., 1989b
Daphnia magna	6 - 24 h old	N	S	Ag	rw	6.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	0.75	2		Cronin et al., 2000
Daphnia magna	6 - 24 h old	N	S	Ag	rw	7.8 ± 0.1	22 ± 2		24 h	EC50	immobilisation	1.76	2		Cronin et al., 2000
Daphnia magna	6 - 24 h old	N	S	Ag	rw	9.0 ± 0.1	22 ± 2		24 h	EC50	immobilisation	11.63	2		Cronin et al., 2000
Daphnia magna		N	S	99 – 100				21.9	24 h	EC50	immobilisation	3.36	2	30	Svenson and Hynning, 1997
Daphnia magna		N		> 98	nw	7	20		48 h	LC50	mortality	0.42	3	31	Kukkonen and Oikari,1987
Daphnia magna		N		> 98	rw	7	20		48 h	LC50	mortality	0.69	2	32	Kukkonen and Oikari, 1987
Daphnia magna	< 72 h old	N	S	> 95	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	5.48	2	33	Devillers and Chambon, 1986a Devillers and Chambon, 1986b Devillers et al., 1987
Daphnia magna	0 - 24 h old	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	48 h	EC50	immobility	3.34	2	22	Holcombe et al., 1987
Daphnia magna									8 d	EC100		5.00	3	34	Schauerte et al., 1982
Daphnia magna	<24h	N	S		rw	8	25	150	48 h	LC50	mortality	6.64	2		Kim et al., 2006
Daphnia magna	< 24 h old	N	S	>98	nw	6.5	20		48 h	LC50	mortality	0.27	3	35,36	Virtanen et al., 1989
Daphnia magna	< 24 h old	N	S	>98	rw	6.5	20		48 h	LC50	mortality	0.33	2	35	Virtanen et al., 1989
Moina macrocopa	ca. 5 d old	N	S	ag	am		20 ± 1		3 h	LC50	mortality	6.03	3	35a	Yoshioka et al., 1986a
Insecta															
Paratanytarsus parthenogeneticus	3rd instar larvae	Y	S		nw	7.4	20	713	48 h	LC50	mortality	47.16	2	37	Meier et al., 2000
Tanytarsus dissimilis	3rd and 4th instar	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	48 h	LC50	mortality	> 13.5	2	22	Holcombe et al., 1987
Pisces															
Carassius auratus	1.0 ± 0.1 g		S	±100	tw	7.0 ± 0.1	27 - 28		5 h	LC50	mortality	4.01	3	39,40	Kishino and Kobayshi, 1996a
Carassius auratus	1.0 ± 0.1 g	N	S	±100	tw	7.0 ± 0.1	27 - 28		2.5 h	LC50	mortality	4.50	3	39	Kishino and Kobayshi, 1996b
Carassius auratus	2.2 ± 0.2 g		S	±100	tw	6	20 - 21		5 h	LC50	mortality	*1.50*	3	39-41	Kishino and Kobayashi, 1995
Carassius auratus	2.2 ± 0.2 g		S	±100	tw	8	20 - 21		5 h	LC50	mortality	*7.00*	3	39-41	Kishino and Kobayashi, 1995
Carassius auratus	2.2 ± 0.2 g		S	±100	tw	10	20 - 21		5 h	LC50	mortality	*> 70*	3	39-41	Kishino and Kobayashi, 1995

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Carassius auratus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	≥ 5	3	42	Wood, 1953
Carassius auratus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	5.00	3	42	Hollis and Lennon, 1954
Carassius auratus	2 g		R				20		24 h	LC50	mortality	10.00	2		Kobayashi et al., 1979
Danio rerio	adults	Y				7.2 - 7.5	24		96 h	LC50	mortality	0.58	2	43	Neilson et al., 1990
Danio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	1.90	2		Devillers and Chambon, 1986
Jordanella floridae	juveniles, 2 - 4 mo, 0.4 - 4 g, 8 - 12% lipid	N	R		dtw	6.95	25 ± 2	48	96 h	LC50	mortality	2.26	2	44	Smith et al., 1991
Jordanella floridae	juveniles, 2 - 4 mo, 0.4 - 4 g, 8 - 12% lipid	Y	F		dtw	6.95	25 ± 2	48	96 h	LC50	mortality	2.21	2	45	Smith et al., 1991
Lepomis macrochirus	0.32 - 1.2 g ww	N	Sc	≥ 80	am	6.5 - 7.9	21 - 23	32 - 48	96 h	LC50	mortality	0.32	2	46,27	Buccafusco et al., 1981
Lepomis macrochirus	fingerlings < 10.2 cm					7	12.8	300	20 h	LOEC	mortality	5.00	3	42	Wood, 1953
Lepomis macrochirus	fingerlings < 10.2 cm					7	12.8	300	24 h	NOEC	mortality	5.00	3	42	Hollis and Lennon, 1954
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		3 h	LOEC	mortality	5.00	3	47	Applegate et al., 1957
Lepomis macrochirus	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		15 h	LOEC	mortality	5.00	3	47	Applegate et al., 1957
Lepomis macrochirus	5.9 g	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	96 h	LC50	mortality	0.41	2	22	Holcombe et al., 1987
Leuciscus idus							20	267	48 h	LC50	mortality	3.00	2		Dietz, 1978
Leuciscus idus melanotus			S			7-8	20	267	48 h	LC50	ortality	1.9	2	65	Rübelt et al., 1982
Oncorhynchus ishawytscha						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	48	MacPhee, 1969
Oncorhynchus ishawytscha						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	48	MacPhee, 1969
Oncorhynchus ishawytscha						7.2 - 7.6			0 - 2.5 h	LOEC	mortality	10.00	4	48	MacPhee, 1969
Oncorhynchus kisutch						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	48	MacPhee, 1969
Oncorhynchus kisutch						7.2 - 7.6			0 - 1 h	LOEC	mortality	10.00	4	48	MacPhee, 1969
Oncorhynchus mykiss	0.9 - 13.1 g	Y	F	98	nw	7.03 - 7.66	16.6 - 17.4	44.7	96 h	LC50	mortality	0.73	4*	49	Sulaiman, 1993
Oncorhynchus mykiss	1 - 5 g	Y	CF	> 99	tw	7.8	15		96 h	LC50	mortality	0.57	2	50	Hodson et al., 1984
Oncorhynchus mykiss	2.3 g	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	96 h	LC50	mortality	0.73	2	22	Holcombe et al., 1987
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		4 h	LOEC	mortality	5.00	3	47	Applegate et al., 1957
Oncorhynchus mykiss	fingerlings, ca. 10 cm	N	S		nw	7.5 - 8.2	13		3 h	LOEC	mortality	5.00	3	47	Applegate et al., 1957
Oryzias latipes			R		tw	7.2	20 ± 1	40	48 h	LC50	mortality	1.50	2	51	Yoshioka and Ose, 1993
Oryzias latipes	ca. 3 cm, 0.3 g	N	S	ag	dw		20 ± 1	80	48 h	LC50	mortality	1.51	2		Yoshioka et al., 1986
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		12 h	LOEC	mortality	5.00	3	47	Applegate et al., 1957
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality	≥ 5	3	47	Applegate et al., 1957
Petromyzon marinus	larvae, 7.6 - 13 cm, collected from the field	N	S		nw	7.5 - 8.2	13		24 h	NOEC	mortality	≥ 5	3	47	Applegate et al., 1957
Pimephales promelas									96 h	LC50	mortality	2.79	4	52	Eldred et al., 1999
Pimephales promelas	30 - 35 d old	Y	F		nw	7.5	25 ± 2	43.3 - 48.5	96 h	LC50	mortality	9.70	2	53	Phipps et al., 1981
Pimephales promelas	30 - 35 d old	Y	F		nw	7.5	25 ± 2	43.3 - 48.5	96 h	LC50	mortality	8.60	2	54	Phipps et al., 1981
Pimephales promelas	30 - 35 d old	Y	F		nw	7.5	25 ± 2	43.3 - 48.5	192 h	LC50	mortality	5.80	2	53	Phipps et al., 1981
Pimephales promelas	30 - 35 d old	Y	F		nw	7.5	25 ± 2	43.3 - 48.5	192 h	LC50	mortality	6.40	2	54	Phipps et al., 1981
Pimephales promelas	30 - 35 d old	Y	S		nw	7.5	21.6 - 25.4	43.3 - 48.5	48 h	LC50	mortality	7.70	2		Phipps et al., 1981
Pimephales promelas	0.2 - 0.4 g	Y	F	98	nw	7.03 - 7.66	16.6 - 17.4	44.7	96 h	LC50	mortality	2.74	4*	55	Sulaiman, 1993
Pimephales promelas	29 d, 18.8 mm, 90 mg	Y	F		nw/ dtw	7.9	24.8	42.6	96 h	LC50	mortality	4.55	1		Geiger et al., 1988
Pimephales promelas	34 d, 0.124 g	Y	F	rg	nw/ dtw	7.52	25.3	46	96 h	LC50	mortality	9.16	1		Geiger et al., 1985
Pimephales promelas		Y	F		nw/ dtw				96 h	LC50	mortality	4.89	4		Geiger et al., 1990

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Pimephales promelas		N	S						24 h	LC50	mortality	3.20	4		Ingols and Gaffney, 1965
Pimephales promelas			S						96 h	LC50	mortality	0.1 - 1	4	56	Kilzer et al., 1979
Pimephales promelas	30 - 35 d		F		nw		25 ± 2	43.3 - 48.5	192 h	LC50	mortality	9.24	4	57	Hall et al., 1984
Pimephales promelas	26 - 34 d old (juveniles), laboratory-cultured	Y	CF	> 95	nw	7.8	25	45	96 h	LC50	mortality	4.55	4*	58	Veith and Broderius, 1987 Broderius et al. 1995
Pimephales promelas	0.2 g	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	96 h	LC50	mortality	2.74	2	22	Holcombe et al., 1987
Poecilia reticulata	40 - 60 mg	Y	R	≥ 99	dw	5 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	0.61	3	59,60	Saarikoski and Viluksela, 1981
Poecilia reticulata	40 - 60 mg	Y	R	≥ 99	dw	6 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	0.89	4*	60	Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg	Y	R	≥ 99	dw	7 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	2.29	4*	60	Saarikoski and Viluksela, 1981
Poecilia reticulata	40 - 60 mg	Y	R	≥ 99	dw	8 ± 0.1	26 ± 0.1	80 - 100	96 h	LC50	mortality	7.86	4*	60	Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg		R			6	26 ± 1		96 h	LC50	mortality	0.88	2		Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg		R			7	26 ± 1		96 h	LC50	mortality	2.27	2		Saarikoski and Viluksela, 1982
Poecilia reticulata	40 - 60 mg		R			8	26 ± 1		96 h	LC50	mortality	7.86	2		Saarikoski and Viluksela, 1982
Poecilia reticulata	2 - 3 mo old males			rg	tw	7.7 ± 0.1			24 h	LC50	mortality	0.46	4	61	Benoit-Guyod et al., 1984
Poecilia reticulata									96 h	LC50	mortality	2.30	4		European Commission (European Chemical Bureau), 2000
Poecilia reticulata	40 - 60 mg	Y	R		dtw	7	25-27		96 h	LC50	mortality	2.20	2	62	Salkinoja-Salonen et al., 1981
Ptychochelilus oregonensis						7.2 - 7.6			0 - 1 h	LOEC	sublethal effects	10.00	4	48	MacPhee, 1969
Ptychochelilus oregonensis						7.2 - 7.6			1 - 3 h	LOEC	mortality	10.00	4	48	MacPhee, 1969. In: Lipnick et al., 1985.
Ptychochelilus oregonensis						7.2 - 7.6			0 - 1 h	LOEC	sublethal effects	10.00	4	48	MacPhee, 1969. In: Lipnick et al., 1985.
Ptychochelilus oregonensis						7.2 - 7.6			1 - 2.5 h	LOEC	mortality	10.00	4	48	MacPhee, 1969. In: Lipnick et al., 1985.
Salmo trutta	average 4.5 g						ca. 5		24 h	LC50	mortality	1.10	2		Hattula et al., 1981
Salmo trutta	fingerlings < 10.2 cm					7	12.8	300	2 h	LOEC	mortality	5.00	3	42	Wood, 1953
Salvelinus fontinalis	fingerlings < 10.2 cm					7	12.8	300	3 h	LOEC	mortality	5.00	3	42	Hollis and Lennon, 1954
Tilapia zilli	2 - 6 cm	N	R	rg		6.6	25 ± 1	215		LC50	mortality	3.73	2	63	Yen et al., 2002
Amphibia															
Xenopus laevis	tadpoles	Y	F		nw	7.39 ± 0.22	17.2 ± 0.5	44.7	96 h	LC50	mortality	1.20	2	22	Holcombe et al., 1987

Notes
1 Species is relevant to the aquatic compartment
2 Mean of three determinations; test duration not clear
3 Test result is average of three replicates; soil bacteria which also occurs in water
4 Exposure time not clear, probably too long for a bacteria test
5 Reported as Minimal Inhibition Concentration (MIC); test duration not celar
6 Original reference unclear; test duration not reported
7 EC50 calculated by fitting a logistic dose response model through data presented by author. EC50 value is slightly extrapolated (highest tested concentration was 10 mg/L).
8 Mutant, which is more sensitive to toxicants than natural strain.
9 Test duration > 96 h and unclear if cells are still in exponential growth phase.
10 Solvent DMSO is not toxic in solvent controls
11 In accordance with US EPA method. ; Test duration too long
12 Details test medium from Bringmann and Kuhn, 1980
13 ≤ 0.7% DMSO. Unclear if the EC50 is based on nominal or mean measured concentrations. Recovery of the test substance was > 80% of nominal in an abiotic control;
15 9 h equals 3 generation times
16 Sealed for volatile compounds; < 5000 mg/l DMSO (non-toxic) for slightly soluble substances; substance name adapted from Yoshioka et al. 1986 (EES)
17 Exposure duration not reported, but in accordance with U.S. EPA (1985).
18 Fronds were considered to be dead when they were colorless over more than half the surface of the bath. Study deemed unreliable because of possible metabolic transformation and lack of measurements.

19 Reported as Minimal Affective Concentration.
20 Criterion (tulip stage) considered relevant because it preceeds desintegration (mortality).
21 Animals were cut in parts; body parts were used for toxicity testing. Similar to growth of animals in the field
22 Test result based on nominal concentrations; measured concentrations were > 80% of nominal. Several species were simultaneously exposed to the test substance in an exposure tank with seperate exposure chambers. Exposure tanks were covered.
23 Test result is based on measured initial concentrations. Although a solvent control was included, it is unclear if a control without solvent was included as well.
24 In accordance with U.S. EPA 1985, ASTM 1988.
25 In accordance with US EPA guidelines. Test result is average of three replicates.
26 Results based on initial concentrations. pH too high (6 - 9 is acceptable according to OECD guideline)
27 In accordance with U.S. EPA (1975).
28 In accordance with ISO (1985).
29 In accordance with DIN 38412, Part II 1982.
30 In accordance with Swedish Standard SS 02 81 80.
31 Natural humic water (DOC = 23.5 mg/L). Hardness reported as 0.1 mM Ca + Mg (unclear if 0.1 mM Ca and 0.1 mM Mg or sum Ca + Mg is 0.1 mM is ment).
32 Control water (no humic acids). Hardness reported as 0.5 mM Ca + Mg (unclear if 0.5 mM Ca and 0.5 mM Mg or sum Ca + Mg is 0.5 mM is ment). .
33 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
34 Field test
35 According to OECD guidelines
35a Exposure time too short
36 natural humic water
37 Based on measured concentrations
39 No control group included.
40 A 5-h exposure period was chosen, because within this period, no detoxification of the test substance occurred.
41 LC50 are only indicative values, because not all concentrations were observed until 5 hours.
42 Reported as time to effect. Only two fish tested.
43 Results based on measured concentrations
44 In accordance with U.S. EPA 1975. Solvent (acetone) not toxic at used concentrations (solvent control included)
45 Unclear if test result is based on nominal or measured concentrations. However, recovery was ≥ 80%. In accordance with U.S. EPA 1975. Solvent (acetone) not toxic at used concentrations (solvent control included)
46 Dissolved oxygen concentrations too low (range: 9.7 at start - 0.3 mg/L after 96 h) for a number of the compounds tested). Not clear if this was also the case for this compound.
47 Only two fish were tested. Reported as time to effect. Up to three fish species were tested simultanuously.
48 Endpoint unclear. Reported as time to effect.
49 Unclear if test result is based on nominal or actual concentrations. Recovery of test substance not reported. Large variation in body weight. Same test as Holcombe?
50 Test result is mean of 3 bioassays. Oxygen concentration may have been low (range of all experiments: 5.6 - 9.4 mg/L O_2 at 14.1 - 16.5 °C).
51 In accordance with OECD 203.
52 COMPUTOX database
53 Replicate 1; According to US EPA methods; Compound was measured but recoveries not reported, also unclear if results are based on measured or nominal concentrations
54 Replicate 2; According to US EPA methods; Compound was measured but recoveries not reported, also unclear if results are based on measured or nominal concentrations
55 Unclear if test result is based on nominal or actual concentrations. Recovery of test substance not reported. Probably the same test as Holcombe
56 Reported as TLm.
57 Unit of endpoint not reported. Assumed that unit is mol/L. In accordance with EPA-660/3-75-009.
58 In accordance with ASTM 1980. Unclear if the LC50 is based on nominal or mean measured concentrations, but recovery of the test substance was > 90% of nominal. Not clear if tested together with phenol or separately
59 pH 5 may be stressful to guppies.
60 Preliminary test showed that in 12 hours, less than 5% of the compound disappeared
61 Unit of LC50 not reported; calculated from log 1/LC50, assuming LC50 is given in mol/L
62 Unclear if results are based on measured or nominal concentrations; measured concentrations close to nominal concentrations
63 Test duration not reported, probably 96 hours.
64 According to standard APHA methods
65 According to standard German test methods (1974)

Table A2.12 Acute toxicity of 2,4,6-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S	> 98					30 min	EC50	bioluminescence	12.7	2	1	Twagilimana et al., 1998
Vibrio fischeri		N	S		am		15	21.9	30 min	EC50	bioluminescence	7.7	2	2	Ribo and Kaiser, 1983
Vibrio fischeri		N	S, open		am	6.5 - 7.5	15		5 min	EC50	bioluminescence	1.9	2	1	Blum and Speece, 1991a Blum and Speece, 1991b
Vibrio fischeri		N	S	97	am	7	15	21.9	15 min	EC50	bioluminescence	10.4	2	1	Svenson and Zhang, 1995
Vibrio fischeri		N	S	97	am	7.3	15	21.9	15 min	EC50	bioluminescence	14.7	2	1	Svenson and Zhang, 1995
Vibrio fischeri								21.9	30 min	EC50	bioluminescence	4.3	2	3	Schüürmann and Segner, 1994
Vibrio fischeri	ahs98 (antibiotic hypersensitive mutant of strain NRRL B-11177 (1.0E+06 cells/mL)				am		20	21.9	30 min	EC50	bioluminescence	71.2	3	4	Wagner et al, 1989
Vibrio fischeri		Y				7.2	15		15 min	EC50	bioluminescence	23	2	1	Neilson et al., 1990
Vibrio fischeri		N	S	99 - 100		7		21.9	15 min	EC50	bioluminescence	6.7	2	1	Svenson and Hynning., 1997
Vibrio fischeri		N	S		am	6.0 - 7.0	20		5 - 60 min	EC50	bioluminescence	14.5	4	1	McDowell and Boardman, 1986
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	22.6	2		Westbury, 1998
Vibrio fischeri		N	S				15		15 min	EC50	bioluminescence	7.1	2		Stauber et al, 1994
Algae															
Glenodinium halli				tg	nw		20	25	7 d	EC50	cell division	4	2		Erickson and Freeman, 1978
Isochrysis galbana				tg	nw		20	25	7 d	EC50	cell division	0.5	2		Erickson and Freeman, 1978
Nitzschia closterium	log growth phase	Y	S				21		72 h	EC50	cell division	10.1	2		Stauber et al., 1994
Skeletonema costatum				tg	nw		20	25	7 d	EC50	cell division	8	2		Erickson and Freeman, 1978
Thalassiosira pseudonana				tg	nw		20	25	7 d	EC50	cell division	4	2		Erickson and Freeman, 1978
Mollusca															
Mya arenaria	ca. 5 cm length, 20 g	Y	R		nw		10	30	96 h	LC50	mortality	3.9	3	5	McLeese et al., 1979
Crustacea															
Palaemonetes pugio	juveniles, < 20 mm, collected from the field	Y	S		nw	6.1 - 8.0	20 ± 2	10 ± 1	48 h	LC50	mortality	5.6	2	6	Burton and Fisher., 1990
Palaemonetes pugio	intermoulting adults, field collected; 25 mm	N	R	98	nw		20	10	96 h	LC50	mortality	3.95	2	7	Rao et al., 1981
Palaemonetes pugio	moulting adults, field collected; 25 mm	N	R		nw		20	10	96 h	LC50	mortality	1.21	2	8	Rao et al., 1981
Pisces															
Fundulus heteroclitus	juveniles, < 23 d old, reared from eggs of adults collected in the field	Y	S		nw	6.1 - 8.0	20 ± 2	10 ± 1	48 h	LC50	mortality	2.3	2	6	Burton and Fisher, 1990
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	1.4	2	9	Smith et al., 1994

Notes
1 Microtox test.
2 Data from 15 and 30 min-exposures are most accurate.
3 In accordance with DIN 38412 L34.
4 EC50 determined from figure using TechDig. Mutagenesis induced by chemical to obtain more sensitive mutant. Unit of EC50 is not reported.
5 Exposure time not fixed (time to lethality experiment). Unclear if LC50 is based on nominal or measured concentrations, but concentrations remained practically constant. 3 shrimp and 3 clams were exposed simultaneously.
6 In accordance with ASTM (1980). Results based on measured concentrations.
7 Intermoult.
8 Moulting.
9 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L), but concentrations are measured and control included. Tightly fitted glass lid, aeration unclear.

Table A2.13 Chronic toxicity of 2,4,6-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	NOEC	maximum growth yield	7.3	2	1	Cenci et al., 1987
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	NOEC	specific growth rate	14.8	2	1	Cenci et al., 1987
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	NOEC	lag time	3.6	2	1,2	Cenci et al., 1987
Escherichia coli	NCTC 9001, 1E+07 cells/mL	N	S		am	7	37		≤ 24 h	NOEC	dehydrogenase activity	14.8	2	1	Cenci et al., 1987
Cyanobacteria															
Anabaena sp.		Y			am	6.8 - 7.2	17			NOEC	growth rate	0.165	2	3,4,5	Neilson et al., 1990
Algae															
Chlorella pyrenoidosa		N	S		am	7	22		72 h	NOEC	chlorophyll/ oxygen production	1	4	6	Huang and Gloyna, 1968
Scenedesmus sp.		Y			am	6.8 - 7.2	17			NOEC	growth rate	0.33	2	4,5,7	Neilson et al., 1990
Scenedesmus subspicatus	ca. 10^4 cells/mL	N	S	98	am	7	22 ± 2	550	96 h	EC10	biomass (AUC)	1.1	2	8	Geyer et al., 1985
Scenedesmus subspicatus		N	S		am	7	27	550	8 d	LOEC	growth	0.197	2	9	Schmidt and Schnabl, 1988
Scenedesmus subspicatus					am	7	27	550	8 d	LOEC	fluorescence	0.20	2	9,10	Schmidt and Schnabl, 1988
Macrophyta															
Lemna perpusilla	single three-frond colony	N	S		am		27		10-14 d	NOEC	growth: frond number	0.1	3	11	Rowe et al., 1982
Lemna perpusilla	single three-frond colony	N	S		am		27		10-14 d	EC100	growth: frond number	5	3	11	Rowe et al., 1982
Fungi															
Saccharomyces cerevisiae	10^7 cells from early stationary culture				am		30		24 h	NOEC	growth	0.0026	4	12	Ahlers et al., 1988
Rotifera															
Brachionus calyciflorus	newly hatched	N	S	98	am	7.5	25		48 h	NOEC	reproduction	0.30	2		Radix et al., 1999
Brachionus calyciflorus	newly hatched	N	S	98	am	7.5	25		48 h	EC10	reproduction	0.42	2		Radix et al., 1999
Brachionus calyciflorus	newly hatched	N	S	98	am	7.5	25		48 h	EC50	reproduction	3.00	2		Radix et al., 1999
Crustacea															
Daphnia magna	< 24 h old	Y	R	98	am	8.5 ± 0.2	20 ± 1	140 - 160	21 d	NOEC	reproduction	0.50	2	13,14	Radix et al., 1999
Insecta															
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	hatchability	5.67	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	hatchability	4.35	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	hatchability	2.68	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	larval development	1.09	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	larval development	1.91	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	larval development	1.79	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	pupal formation	0.99	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	pupal formation	1.74	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	pupal formation	1.65	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult emergence	0.77	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult emergence	1.65	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult emergence	1.57	1	15	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC10	adult survival	0.39	2	14,16	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult survival	1.52	2	14,16	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC10	adult survival	0.92	2	14,16	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult survival	1.96	2	14,16	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC10	adult survival	0.56	2	14,16	Meier et al., 2000
Paratanytarsus parthenogeneticus	eggs	Y	F		nw	7.4	20	713	19 - 22 d	EC50	adult survival	1.89	2	14,16	Meier et al., 2000

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Pisces															
Jordanella floridae	fertilised eggs < 24 h old	Y	F		dtw	6.95	25 ± 1	48	10 d p.h.	EC10	hatching success	1.46	2	16,17,18	Smith et al., 1991
Jordanella floridae	fertilised eggs < 24 h old	Y	F		dtw	6.95	25 ± 1	48	10 d p.h.	NOEC	larval survival	≥ 1.766	2	16,17,18	Smith et al., 1991
Jordanella floridae	1-week old fry	Y	F		dtw	6.95	25 ± 1	48)	28 d	EC10	survival	1.43	2	18	Smith et al., 1991
Jordanella floridae	1-week old fry	Y	F		dtw	6.95	25 ± 1	48	28 d	EC10	growth (wwt)	0.089	3	16,18,19,20	Smith et al., 1991
Oncorhynchus mykiss	fertilised eggs < 24 h old	S			rw	7.4-8.05	10		13 d	NOEC	hatching	<0.2	2	21	Freitag et al., 1991
Oncorhynchus mykiss	fertilised eggs < 24 h old	S			rw	7.4-8.05	10		13 d	NOEC	deformations	<0.2	2	22	Freitag et al., 1991
Pimephales promelas	embryos	Y	F						until hatching	NOEC	embryo hatching	2.1	2	23	LeBlanc, 1984
Pimephales promelas	larvae	Y	F						30 d p.h.	NOEC	survival	0.97	2	23,24	LeBlanc, 1984
Pimephales promelas	larvae	Y	F						30 d p.h.	NOEC	growth	0.97	2	23,24	LeBlanc, 1984

Notes
1 Exposure time not clear.
2 Lag time is defined as the time (h) required to attain the mid-point of the growth curve.
3 Calculated from EC20: NOEC = 0.33 / 2.
4 Exposure duration not reported, but in accordance with OECD (1984).
5 Results based on measured concentrations
6 Cell densitiy too high
7 Calculated from EC20: NOEC = 0.65 / 2.
8 Details testmedium from Bringmann and Kuhn
9 Reported as an IC10, which was defined as the lowest concentration that differs statistically from the control and thus an unknown % effect.
10 Relevant endpoint since chlorophenols uncouple electron transport
11 Concentration does not stay constant in static system for 14 days
12 Calculated using EC20: NOEC = 0.00516 / 2. Unit test result unclear.
13 Recovery is not reported. In accordance with OECD 202 993).
14 Test result based on nominal concentrations.
15 Based on mean measured concentrations
16 Endpoint calculated by fitting a logistic dose response model through data presented by author.
17 Exposure duration 10 days post hatching.
18 Solvent (acetone) not toxic at used concentrations (solvent control included)
19 According to authors, NOEC = 0.542 mg/L, but a significant decrease was also seen at a lower test concentration (no clear dose-response curve).
20 EC10 extrapolated a factor 2 below the lowest test concentration.
21 50% effect at 0.2 mg/L; 0.2 mg/L was only concentration tested.
22 74% effect at 0.2 mg/L; 0.2 mg/L was only concentration tested.
23 In accordance with US EPA 1972.
24 Exposure duration 30 d post hatching

Table A2.14 Chronic toxicity of 2,4,6-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S	98	am	7.5	27	38.4	22 h	NOEC	bioluminescence	0.05	2	1	Radix et al., 1999
Vibrio fischeri		N	S	98	am	7.5	27	38.4	22 h	EC10	bioluminescence	0.054	2	1	Radix et al., 1999
Vibrio fischeri		N	S	98	am	7.5	27	38.4	22 h	EC50	bioluminescence	0.165	2	1	Radix et al., 1999
Algae															
Field community		F	tg		am		12	20	24 h	NOEC	14C uptake	>2.0	3	2	Erickson and Hawkins, 1980
Nitzschia sp.		Y			am	6.8 - 7.2	17			NOEC	growth rate	0.28	2	3	Neilson et al., 1990
Nitzschia closterium	log growth phase	Y	S				21		72 h	LOEC	cell division	1.97	2	4	Stauber et al., 1994

Notes
1 Microtox chronic toxicity test.
2 Field community; species not defined
3 Calculated from EC20: NOEC = 0.56 / 2. Exposure duration not reported, but in accordance with OECD (1984). Results based on measured concentrations.
4 Lowest test concentration.

Table A2.15 Acute toxicity of 3,4,5-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Bacillus sp.	isolated from activated sludge, cell age 18 - 20 h						21		30 min	EC50	dehydrogenase activity	5.00	2	1	Liu et al., 1982
Burkholderia RASC c2	*lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	0.87	2	2	Boyd et al., 2001
Pseudomonas fluorescens	soil bacteria, *lux*-marked, Gram-negative	N	S	≥ 98	am	7.1	25		20 min	EC50	bioluminescence	1.88	2	3	Boyd et al., 2001
Cnidaria															
Hydra vulgaris	adult	N	R	purified	am	7			44 h	LOEC	tulip stage	1.00	2	4	Mayura et al., 1991
Macrophyta															
Lemna minor		Y		> 98	am	6.8 - 7.2	17			EC50	yield (dry weight)	0.32	2	5	Neilson et al., 1990
Crustacea															
Ceriodaphnia dubia		Y		> 98		7.9 - 8.1	25		48 h	LC50	mortality	0.39	2	6	Neilson et al., 1990
Daphnia magna		Y		> 98		7.9 - 8.1	20		48 h	LC50	mortality	0.68	2	6	Neilson et al., 1990
Daphnia magna	< 72 h old	N	S	> 95	rw	7.8 - 8.2	20 ± 1	200	24 h	EC50	immobility	0.88	2	7	Devillers and Chambon, 1986a Devillers and Chambon, 1986b Devillers et al., 1987
Nitocra spinipes	copepod	Y		> 98		7.9 - 8.1	20		48 h	LC50	mortality	0.40	2	8	Neilson et al., 1990
Pisces															
Danio rerio	adults	Y		> 98		7.2 - 7.5	24		96 h	LC50	mortality	0.44	2	8	Neilson et al., 1990
Danio rerio	larvae	Y	R	> 98		7.2 - 7.5	24		96 h	LC50	survival	0.20	2	8	Neilson et al., 1990
Danio rerio	160 - 185 mg	N		> 95	am		22 ± 1		24 h	LC50	mortality	0.97	2		Devillers and Chambon, 1986b
Poecilia reticulata	2 - 3 mo		R		am or rw	6.1	22 ± 1	25	7 or 14 d	LC50	mortality	1.14	2	9	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo		R		am or rw	7.3	22 ± 1	25	7 or 14 d	LC50	mortality	1.14	2	9	Könemann and Musch, 1981
Poecilia reticulata	2 - 3 mo		R		am or rw	7.7 - 7.9	22 ± 1	25	7 or 14 d	LC50	mortality	2.37	2	9	Könemann and Musch, 1981

Notes
1 Species is relevant to the aquatic compartment.
2 Test result is average of three replicates.
3 Test result is average of three replicates; soil bacteria which also occurs in water
4 Criterion (tulip stage) considered relevant because it preceeds desintegration (mortality).
5 Exposure duration not reported, but in accordance with U.S. EPA (1985). Results based on measured concentrations
6 In accordance with ISO (1985). Results based on measured concentrations
7 Test performed in closed system; test was considered valid when dissolved oxygen concentration ≥ 2.27 mg/L which is slightly lower than the oxygen level given in OECD 202 (≥ 3 mg/L).
8 Results based on measured concentrations
9 Exposure duration (7 or 14 days) not clear; influence of pH on toxicity tested.

Table A2.16 Acute toxicity of 3,4,5-trichlorophenol to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri		N	S		am		15	21.9	30 min	EC50	bioluminescence	0.36	2	1	Ribo and Kaiser, 1983
Vibrio fischeri		N	S	98	am	7	15	21.9	15 min	EC50	bioluminescence	0.34	2	1	Svenson and Zhang, 1995
Vibrio fischeri		N	S	98	am	7.3	15	21.9	15 min	EC50	bioluminescence	0.39	2	1	Svenson and Zhang, 1995
Vibrio fischeri		Y		> 98		7.2	15		15 min	EC50	bioluminescence	0.47	2	1	Neilson et al., 1990
Pisces															
Platichthys flesus	collected in the field, 56 ± 2.5 g	Y	R	≥ 98		8 ± 0.1	6	5	96 h	LC50	mortality	2.31	2	2	Smith et al., 1994

Notes
1 Microtox test.
2 In accordance with OECD 203 (1981). Fish loading exceeds recommended value (34 g/L instead of 1 g/L), but concentrations are measured and control included. Tightly fitted glass lid, aeration unclear

Table A2.17 Chronic toxicity of 3,4,5-trichlorophenol to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness $CaCO_3$ [mg/L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Scenedesmus sp.		Y		> 98	am	6.8 - 7.2	17			NOEC	growth rate	0.145	2	1	Neilson et al., 1990
Nitzschia sp.		Y		> 98	am	6.8 - 7.2	17			NOEC	growth rate	0.06	2	2	Neilson et al., 1990
Anabaena sp.		Y		> 98	am	6.8 - 7.2	17			NOEC	growth rate	0.175	2	3	Neilson et al., 1990
Pisces															
Danio rerio	eggs	Y	R	> 98						LOEC	median larval survival time	0.05	4	4	Neilson et al., 1990
Danio rerio	eggs	Y	R	> 98						LOEC	deformation frequency	0.09	4	4	Neilson et al., 1990
Danio rerio	eggs	Y	R	> 98					See note	NOEC	median larval survival time, deformation frequency	0.05	4	5	Neilson et al., 1990
Danio rerio	eggs	Y	R	> 98					See note	LOEC	median larval survival time, deformation frequency	0.07	4	5	Neilson et al., 1990

Notes
1 Calculated from EC20: NOEC = 0.29 / 2. Exposure duration not reported, but in accordance with OECD (1984). Based on measured data
2 Calculated from EC20: NOEC = 0.12 / 2. Exposure duration not reported, but in accordance with OECD (1984). Based on measured data
3 Calculated from EC20: NOEC = 0.35 / 2. Exposure duration not reported, but in accordance with OECD (1984). Based on measured data
4 ELS test. LOEC arbitrarily chosen as concentration where > 10% effect was observed. Test duration not reported, but duration covers development from eggs to larvae.
5 modified Eggs used were from adults that were exposed for 6 wk and held in dilution water (without test substance) for another 6 wk (eggs were exposed as well: pre/post-exposure was followed by normal embryo/larvae test). Reported is geometric mean of 14 NOECs during 3 years of testing

rivm

Appendix 3. Bird and mammal toxicity data

Table A3.1 Bird and mammal toxicity data of 2,4,6-trichlorophenol.

Species	Species properties	purity	Application route[b]	Exposure time	Criterion	Test endpoint[b]	Effect concentration [mg/kg$_{bw}$/day]	Effect concentration [mg/kg$_{diet}$]	Effect concentration [mg/L]	Ri	Notes	Reference
rat	Sprague-Dawley		oral; not specified	90 d	NOAEL	liver toxicity	80			3	1	EC, 2000
rat			drinking water	2 year		reproduction				3	2	EC, 2000
rat	F844; 6 w old		diet	106-107 weeks	NOAEL	body weight; carcinogenicity	<5000			2	3	EC, 2000
mouse	C57BL		first gavage, then diet	78 weeks	NOAEL	carcinogenicity	>260			3	4	EC, 2000
mouse	B6C3F1		diet	105 weeks	NOAEL	carcinogenicity; body weight	<5000			2		EC, 2000
rat			oral; not specified	2 years	ECx	carcinogenicity	185			4	5	EC, 2000
rat			oral; not specified	2 years	ECx	carcinogenicity	374			4	5	EC, 2000
mouse			oral; not specified	2 years	ECx	carcinogenicity	441			4	5	EC, 2000
mouse			oral; not specified	2 years	ECx	carcinogenicity	882			4	5	EC, 2000
rat	female, Long-Evans		gavage	2 weeks pre-mating and through gestation	NOAEL	maternal survival and body weight	**500**			2		EC, 2000
rat	female, Long-Evans		gavage	2 weeks pre-mating and through gestation	NOAEL	birth weight	**100**			2		EC, 2000
rat	male, Long-Evans		gavage	10 weeks	NOAEL	copulatory behaviour; sperm quality	> 1000			2		EC, 2000
rat	Sprague-Dawley; female		drinking water	3 weeks	NOAEL	litter size			30	2		EC, 2000
rat	Sprague-Dawley; female		drinking water	24 months	NOAEL	teratogenicity			< 3	2		EC, 2000
rat	Long-Evans, males		gavage	10 weeks	NOAEL	sperm quality; fertility	> 1000			2		EC, 2000
rat	Long-Evans, females		gavage	2 weeks pre-mating and through gestation	NOAEL	maternal survival	500			4*		EC, 2000
rat	Long-Evans, females		gavage	2 weeks pre-mating and through gestation	NOAEL	birth weight	100			4*		EC, 2000

[a] Studies with irrelevant application routes (single oral gavage, dermal, intraperitoneal, etc.) not included
[b] Studies with irrelevant endpoints (for instance, ChE activity) not included

Notes
1 Endpoint not valid
2 Reproduction affected, but test concentrations not specified
3 5000 ppm was the lowest concentration tested
4 Exposure during the first 4 weeks by gavage, after that by diet
5 unclear if result is given in mg/kg$_{bw}$/d or mg/kg diet

Appendix 4. References used in the appendices

Ahlers J, Benzing M, Gies A, Pauli W, Roesick E. 1988. Yeast - an unicellular model system in ecotoxicology and xenobiochemistry. Chemosphere 17: 1603-1615.

Applegate VC, Howell JH, Hall AE Jr., Smith AM. 1957. Toxicity of 4,346 chemicals to larval lampreys and fishes. Washinghton DC, USA: U.S. Fish and Wildlife Services, Department of the Interior. Special scientific report, Fisheries No. 207.

Arthur AD, Dixon DG. 1994. Effects of rearing density on the growth response of juvenile fathead minnow (*Pimephales promelas*) under toxicant-induced stress. Can J Fish Aquat Sci 51: 365-371.

Azim F. 1998. Models to predict the toxicity of polar narcotic chemicals to Daphnia carinata. Honours Thesis, University of Technology Sydney, Sydney, Australia.

Banerjee S. 1987. Interrelationship between biodegradability, toxicity, and structure of chlorophenols. In: Kaiser KLE, ed. QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd. Reidel. p. 17-23.

Belfroid AC, Sijm DTHM, Van Gestel CAM. 1996. Bioavailability and toxicokinetics of hydrophobic aromatic compounds in benthic and terrestrial invertebrates. Environ Rev 4: 276-299.

Benoit-Guyod J-L, Andre C, Taillandier G, Rochat J, Boucherle A. 1984. Toxicity and QSAR of chlorophenols on *Lebister reticulatus*. Ecotoxicol Environ Saf 8: 227-235.

Bitton G, Rhodes K, Koopman B. 1996. Ceriofast(TM): an acute toxicity test based on *Ceriodaphnia dubia* feeding behavoir. Environ Toxicol Chem 15: 123-125.

Bitton G, Rhodes K, Koopman B, Cornejo M. 1995. Short-term toxicity assay based on daphnid feeding behavior. Wat Environ Res 67: 290-293.

Blackman, Parka, Garton. 1955. The physiological activity of substituted phenols - I. Relationships between chemical structure and physiological activity. Arch Biochem Biophys 54: 45-54.

Blum DJW, Speece RE. 1991a. A database of chemical toxicity to environmental bacteria and its use in interspecies comparisons and correlations. Research Journal - Water Pollution Control Federation 63: 198-207.

Blum DJW, Speece RE. 1991b. Quantitative structure-activity relationships for chemical toxicity to environmental bacteria. Ecotoxicol Environ Saf 22: 198-224.

Bogaerts P, Senaud J, Bohatier J. 1998. Bioassay technique using nonspecific esterase activities of *Tetrahymena pyriformis* for screening and assessing cytotoxicity of xenobiotics. Environ Toxicol Chem 17: 1600-1605.

Boyd EM, Killham K, Meharg AA. 2001. Toxicity of mono-, di- and tri-chlorophenols to lux marked terrestrial bacteria, *Burkholderia* species Rasc c2 and *Pseudomonas fluorescens*. Chemosphere 43: 157-166.

Bringmann G, Kühn R. 1982. Ergebnisse der Schadwirkung wassergefaehrdender Stoffe gegen *Daphnia magna* in einem weiterenentwickelten standardisierten Testverfahren. Z Wasser-Abwasser-Forsch 15: 1-6.

Broderius SJ, Kahl MD, Hoglund MD. 1995. Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environ Toxicol Chem 14: 1591-1605.

Bryant SE, Schultz TW. 1994. Toxicological assessment of biotransformation products of pentachlorophenol: *Tetrahymena* population growth impairment. Arch Environ Contam Toxicol 26: 299-303.

Buccafusco RJ, Ells SJ, LeBlanc GA. 1981. Acute toxicity of priority pollutants to bluegill (Lepomis macrochirus). Bull Environ Contam Toxicol 26: 446-452.

Burton DT, Fisher DJ. 1990. Acute toxicity of cadmium, copper, zinc, ammonia, 3,3'-dichlorobenzidine, 2,6-dichloro-4-nitroaniline, methylene chloride, and 2,4,6-trichlorophenol to juvenile grass shrimp and killifish. Bull Environ Contam Toxicol 44: 776-783.

Call DJ, Brooke LT, Lu P-Y. 1980. Uptake, elimination and metabolism of three phenols by fathead minnows. Arch Environ Contam Toxicol 9: 699-714.

Carlberg GE, Martinsen K, Kringstad A, Gjessing E, Grande M, Källqvist, SkÍre JU. 1986. Influence of aquatic humus on the biovailability of chlorinated micropullutants in atlantic salmon. Arch Environ Contam Toxicol 15: 543-548.

Cenci G, Caldini G, Morozzi G. 1987. Chlorinated phenol toxicity by bacterial and biochemical tests. Bull Environ Contam Toxicol 38: 868-875.

Cronin MTD, Zhao YH, Yu RL. 2000. pH-dependence and QSAR analysis of the toxicity of phenols and anilines to *Daphnia magna*. Environ Toxicol 15: 140-148.

Devillers J, Chambon P. 1986a. Acute toxicity and QSAR of chlorophenols on *Daphnia magna*. Bull Environ Contam Toxicol 37: 599-605.

Devillers J, Chambon P. 1986b. Acute toxicity of chlorophenols to *Daphnia magna* and *Brachydanio rerio*. J. Fr. Hydrol. 17: 111-119.

Devillers J, Chambon P, Zakarya D, Chastrette M, Chambon R. 1987. A predictive structure-toxicity model with Daphnia magna. Chemosphere 16: 1149-1163.

Dietz F, Traud J. 1978. Geruchs- und Geschmacks-Schwellen-Konzentrationen von Phenolkorpern. gwf-wasser/abwasser 119: 318-325.

Dojlido JR. 1979. Investigations of biodegradability and toxicity of organic compounds. US Environmental Protection Agency. Report no. EPA-600/2-79-163 (NTIS PB80 179336).

Eldred DV, Weikel CL, Jurs PC, Kaiser KLE. 1999. Prediction of Fathead Minnow Acute Toxicity of Organic Compounds from Molecular Structure. Chem Res Toxicol 12: 670-678.

Englund VPM, Heino MP. 1996. The freshwater mussel (*Anodonta anatina*) in monitoring of 2,4,6-treichlorophenyl: behaviour and environmental variation considered. Chemosphere 32: 391-403.

Erickson SJ, Freeman AE. 1978. Toxicity screening of fifteen chlorinated and brominated compounds using four species of marine phytoplankton. 307-310.

Erickson SJ, Hawkins CE. 1980. Effects of halogenated organic compounds on photosynthesis in estuarine phytoplankton. Bull Environ Contam Toxicol 24: 910-915.

European Commission (European Chemical Bureau). 2000. IUCLID (International Uniform Chemical Information Database) on CD-ROM. European Chemicals Bureau, Ispra, Italy.

Freitag D, Geyer H, Kraus A, Viswanathan R, Kotzias D, Attar A, Klein W, Korte F. 1982. Ecotoxicological profile analysis. VII. Screening chemicals for their environmental behavior by comparative evaluation. Ecotoxicol Environ Saf 6: 60-81.

Freitag D, Haas-Jobelius M, Yiwei Y. 1991. Influence of 2,2'-dichlorobiphenyl and 2,4,6-trichlorophenol on development of rainbow trout eggs and larvae. Toxicol Environ Chem 31-32: 401-408.

Freitag D, Lay JP, Korte Freidhelm. 1984. Environmental hazard profile - test results as related to structures and translation into the environment. QSAR in Environmental Toxicology 111-136.

Froehner K, Meyer W, Grimme LH. 2002. Time-dependent toxicity in the long-term inhibition assay with Vibrio fischeri. Chemosphere 46: 987-997 .

Fu LJ, Johnson EM, Newman LM. 1990. Prediction of the developmental toxicity hazard potential of halogenated drinking water disinfection by-products tested by the in vitro hydra assay. Regul Toxicol Pharmacol 11: 213-219.

Geiger DL, Call DJ, Brooke LT Eds. 1988. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*), Vol. 4. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI, USA, 355 pp.

Geiger DL, Northcott CE, Call DJ, Brooke LT, Eds. 1985. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*). Vol. 2. Superior, Wisconsin, USA: Center for Lake Superior Environmental Studies. 326 pp.

Geiger, DL., Brooke LT, Call, DJ, Eds. 1990. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 5. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI, USA.

German Chemical Society (Gesellschaft Deutscher Chemiker). 1994. 2,3-dichlorophenol, BUA Report 110 (June 1991). 2,4,5-trichlorophenol, BUA Report 111 (December 1992). GDCh-Advisory Committee on

Existing Chemicals of Environmental Relevance (BUA). Stuttgart, Germany: S. Hirzel Wissenschaftliche Verlagsgesellschaft. 67 pp.
Geyer H, Politzki G, Freitag D. 1984. Prediction of ecotoxicological behaviour of chemicals: Relationship between n-octanol/water partition coefficient and bioaccumulation of organic chemicals by alga Chlorella. Chemosphere 13: 269-284.
Geyer H, Scheunert I, Korte F. 1985. The effects of organic environmental chemicals on the growth of the alga Scenedesmus subspicatus: a contribution to environmental biology. Chemosphere 14: 1355-1369.
Guerra WKW, Lochmann ER. 1988. Effects of 2,4,5- and 2,4,6-trichlorophenol on growth, RNA-, DNA-, protein-, and ribosome synthesis in Saccharomyces cells. Chemosphere 17: 101-109.
Hall KJ, Jacob C. 1988. Bioconcentration of chlorophenols by leeches and their use as in situ biological monitors. Water Pollut. Res. J. Can. 23: 69-87.
Hall LH, Kier LB, Phipps G. 1984. Structure-activity relationship studies on the toxicities of benzene derivatives: I. an additivity model. Environ Toxicol Chem 3: 355-365.
Hattula ML, Wasenius VM, Reunanen H, Arstila AU. 1981. Acute toxicity of some chlorinated phenols, catechols and cresols to trout. Bull Environ Contam Toxicol 26: 295-298.
Heinonen J, Kukkonen JVK, Holopainen IJ. 2000. Toxicokinetics of 2,4,5-trichlorophenol and benzo(a)pyrene in the clam *Pisidium amnicum*: effects of seasonal temperatures and trematode parasites. Arch Environ Contam Toxicol 39: 352-359.
Heitmuller PT, Hollister TA, Parrish PR. 1981. Acute toxicity of 54 industrial chemicals to sheepshead minnows (*Cyprinodon veriegatus*). Bull Environ Contam Toxicol 27: 596-604.
Hodson PV, Dixon DG, Kaiser KLE. 1984. Measurement of median lethal dose as a rpid indication of contaminant toxicity to fish. Environ Toxicol Chem 3: 243-254.
Holcombe GW, Phipps GL, Sulaiman AH, Hoffman AD. 1987. Simultaneous multiple species testing: acute toxicity of 13 chemicals to 12 diverse freshwater amphibian, fish, and invertebrate families. Arch Environ Contam Toxicol 16: 697-710.
Hollis EH, Lennon RE. 1954. The toxicity of 1085 chemicals to fish. Leetown, West Viriginia: U.S. fish and wildlife service.
Huang J-C, Gloyna EF. 1968. Effects of organic compounds on photosynthetic oxygenation-I. Chlorophyll destruction ans suppression of photosynthetic oxygen production. Water Res 2: 347-366.
Ingols RS, Guffney PE. 1965. Biological Studies of Halophenols. Proc. 14th South. Water Res. Poll. Conf. 14: 175-181.
Jennings JG, De Nys R, Charlton TS, Duncan MW, Steinberg PD. 1996. Phenolic compounds in the nearshore waters of Sydney, Australia. Mar Freshw Res 47: 951-959.
Jones, HR. 1971. Environmental control in the organic and petrochemical industries. Noyes Data Corporation.
Kaila K, Saarikoski J. 1977. Toxicity of penrachlorophenol and 2,3,6-trichlorophenol to the crayfish (*Astacus fluviatilis* L.). Environ Pollut 12: 119-123.
Kilzer L, Scheunert I, Geyer H. 1979. Laboratory Screening of the Volatilization Rates of Organic Chemicals from Water and Soil. Chemosphere 8: 751-761.
Kim KT, Lee YG, Kim SD. 2006. Combined toxicity of copper and phenol derivatives to *Daphnia magna*: effect of complexation reaction. Environ Internat 32: 487-492.
Kishino T, Kobayashi K. 1995. Relation between toxicity and accumulation of chlorophenols at various pH, and their absorption mechanism in fish. Water Res 29: 431-442.
Kishino T, Kobayashi K. 1996a. Acute toxicity and structure-activity relationships of chlorophenols in fish. Water Res 30: 387-392.
Kishino T, Kobayashi K. 1996b. Studies on the mechanism of toxicity of chlorophenols found in fish through quantitative structure-activity relationships. Water Res 30: 393-399.
Klamer HJC, Beekman M. 1995. Estimating the 1-octanol/water partition coefficients (Kow) and fish bioconcentration factors (BCF) of unknown compounds using a gradient HPLC method. Toxicology Modeling 1: 169-179.

Knie J, A. Halke IJ, W. Schiller. 1983. Ergebnisse der untersuchungen von chemischen stoffen mit vier biotests. Deutsche Gewass. Mitt. 3: 77-79.
Kobayashi K, H. Akitake, K. Manabe. 1979. Relation between toxicity and accumulation of various chlorophenols in goldfish. Bull Jap Soc Sci Fish 45: 173-175.
Könemann H, Musch A. 1981. Quantitative structure-activity relationship in fish toxicity studies. Part 2: the influence of pH on the QSAR of chlorophenols. Toxicology 19: 223-228.
Korte F. 1990. Effects and consequences of anthropogenic substances. In: Anonymus GSF-Ber., Proc.-Int. Workshop Study Predict. Pestic. Behav. Soils, Plants Aquat. Sys. p. 1-18.
Korte F, Freitag D, Geyer H, Klein W, Kraus AG, Lahaniatis E. 1978. Ecotoxicological Profile Analysis. A concept for establishing ecotoxicological priority lists for chemicals. Chemosphere 1: 79-102.
Kühn R, Pattard M. 1990. Results of the harmful effects of water pollutants to green algae (*Scenedesmus subspicatus*) in the cell multiplication inhibition test. Water Res 24: 31-38.
Kühn R, Pattard M, Pernak KD, Winter A. 1989a. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Res 23: 495-499.
Kühn R, Pattard M, Pernak KD, Winter A. 1989b. Results of the harmful effects of water pollutants to Daphnia magna in the 21 day reproduction test. Water Res 23: 501-510.
Kukkonen A, Oikari A. 1987. Effects of aquatic humus on accumulation and acute toxicity of some organic micropollutants. Sci Total Environ 62: 399-402.
Kukkonen JVK. 2002. Lethal body residue of chlorophenols and mixtures of chlorophenols in benthic organisms. Arch Environ Contam Toxicol 43: 214-220.
Kwasniewska K, Kaiser KLE. 1983. Toxocities of selected phenols to fermentative and oxidative yeasts. Bull Environ Contam Toxicol 31: 188-194.
LeBlanc GA. 1984. Comparative structure-toxicity relationships between acute and chronic effects to aquatic organisms. QSAR in Environmental Toxicology 235-260.
LeBlanc GA, Hilgenberg B, Cochrane BJ. 1988. Relationships between the structures of chlorinated phenols, their toxicity, and their ability to induce glutathione S-transferase activity in Daphnia magna. Aquat Toxicol 12: 147-155.
Lee HJ, Yoo SO, Lee JG, Kim BY, Chun UH. 1999. Prediction of EC50 of Photobacterium phosphoreum for CAHs and chlorophenol derivatives using QSAR. Sanop Misaengmul Hakhoechi 27 : 54-61.
Lipnick RL, Bickings CK, Johnson DE, Eastmond DA. 1985. Comparison of QSAR predictions with fish toxicity screening data for 110 phenols. ASTM STP 891: 153-176.
Liu D, Thomson K, Kaiser KLE. 1982. Quantitative structure-toxicity relationship pf halogenated phenols on bacteria. Bull Environ Contam Toxicol 29: 130-136.
Lu X, Tao S, Hu H, Dawson RW. 2000. Estimation of bioconcentration factors of nonionic organic compounds in fish by molecular connectivity indices and polarity correction factors. Chemosphere 41: 1675-1688.
MacPhee C, Ruelle R. 1969. Lethal effects of 1,888 chemicals upon four species of fish from western North America. Bulletin 3. Moscow, ID: University of Idaho, Forest Wildlife, and Range Experiment Station. 112 pp.
Makela TP, Petanen T, Kukkonen J, Oikari OJ. 1991. Accumulation and depuration of chloronated phenolics in the freshwater mussel (*Anodonta anatina* L.). Ecotoxicol Environ Saf 22: 153-163.
Mayura K, Smith EE, Clement BA, Phillips TD. 1991. Evaluation of the developmental toxicity of chlorinated phenols utilizing Hydra attenuata and postimplantation rat embryos in culture. Toxicol Appl Pharmacol 108: 253-266.
McDowell AS, Boardman GD. 1986. Three screening tests for the evaluation of groundwater quality. In: Boardman GD, ed. Toxic Hazard. Wastes, Proc. Mid-Atl. Ind. Waste Conf., 18th. Lancaster: Technomic. p. 472-488.
McLeese DW, Zitko V, Peterson MR. 1979. Structure-lethality relationship for phenols, anilines and other aromatic compounds in shrimp and clams. Chemosphere 2: 53-57.
Mulhall A-M. 1997. Models to predict the toxicity of selected phenols and benzamines to a cladoceran and a

marin bacterium. Honours Thesis, University of Technology Sydney, Sydney, Australia.
Meier PG, Choi K, Sweet LI. 2000. Acute and chronic life cycle toxicity of acenaphthene and 2,4,6-trichlorophenol to the midge Paratanytarsus parthenogeneticus (Diptera: Chironomidae). Aquat Toxicol (Amst) 51: 31-44.
Neilson AH, Allard AS, Fischer S, Malmberg M, Viktor T. 1990. Incorporation of a subacute test with zebra fish into a hierarchical system for evaluating the effect of toxicants in the aquatic environment. Ecotoxicol Environ Saf 20: 82-97.
Nendza M, Seydel JK. 1988a. Quantitative structure-toxicity relationships and multivariate data analysis for ecotoxic chemicals in different biotest systems. Chemosphere 17: 1575-1584.
Nendza M, Seydel JK. 1988b. Quantitative structure-toxicity relationships for ecotoxicologically relevant biotest systems and chemicals. Chemosphere 17: 1585-1602.
Nendza M, Seydel JK. 1990. Application of bacterial growth kinetics to in vitro toxicity assessment of substituted phenols and anilines. Ecotoxicol Environ Saf 19: 228-241.
Norberg-King T. 1989. An evaluation of the fathead minnow seven-day subchronic test for estimating chronic toxicity. Environ Toxicol Chem 8: 1075-1089.
Palau CA, Hutchinson TH. 1998. Acute toxicity of chlorinated organic chemicals to the embryos and larvae of the marine worm Platynereis dumerilii (Polychaeta: Nereidae). Environ Toxicol Water Qual 13: 149-155.
Phipps GL, Holcombe GW, Fiandt JT. 1981. Acute toxicity of phenol and sunstituted phenols to the fathead minnow. Bull Environ Contam Toxicol 26: 585-593.
Pill KG, Kupillas GE, Picardal FW, Arnold RG. 1991. Estimating the toxicity of chlorinated organic compounds using a multiparameter bacterial bioassay. Environ Toxicol Water Qual 6: 271-291.
Radix P, Leonard M, Papantoniou C, Roman G, Saouter E, Gallotti SS, Thiebaud H, Vasseur P. 1999. Comparison of *Brachionus calyciflorus* 2-d and Microtox(R) chronic 22-h tests with *Daphnia magna* 21-d test for the chronic toxicity assessment of chemicals. Environ Toxicol Chem 18: 2178-2185.
Rao KR, Fox FR, Conklin PJ, Cantelmo AC. 1981. Comparative toxicology and pharmacology of chlorophenols: studies on the grass shrimp, *Palaemonetes pugio*. Biological Monitoring of Marine Pollutants 37-72.
Ribo JM, Kaiser KLE. 1983. Effects of selected chemicals to photoluminescent bacteria and their correlationswith acute and sublethal effects on other organisms. Chemosphere 12: 1421-1442.
Ribo JM, Rogers F. 1990. Toxicity of mixtures of aquatic contaminants using the luminescent bacteria bioassay. Toxicity Assessment 5: 135-152.
Rowe EL, Ziobro RJ, Wang CJK, Dence CW. 1982. The use of an algae *Chlorella pyrendoidosa* and a duckweed *Lemna perpusilla* as test organisms for toxicity bioassays of spent bleaching liquors and their components. Environ Pollut (Ser A) 27: 289-296.
Rübelt C, Dietz F, Kickuth R, Koppe P, Kunte H, Pescherl G, Sonneborn M. 1982. Schadstoffe im Wasser, Band II, Phenole. Chapter 5: Biologische Wirksamkeit. pp 101-115. Boppard: Harald Boldt Verlag.
Saarikoski J, Viluksela M. 1981. Influence of pH on the toxicity of substituted phenols to fish. Arch Environ Contam Toxicol 10: 747-753.
Saarikoski J, Viluksela M. 1982. Relation between physicochemical properties of phenols and their toxicity and accumulation in fish. Ecotoxicol Environ Saf 6: 501-512.
Salkinoja-Salonen M, Saxelin M-L, Pere J, Jaakkola T, Saarikoski J, Hakulinen R, Koistinen O. Chapter 56: Analysis of toxicity and biodegradability of organochlorine compounds released into the environment in bleaching effluent of kraft pulping. Industrial wastewater analysis. p. 1131-1164.
Schauerte W, Lay JP, Klein W, Korte F. 1982. Influence of 2,4,6-trichlorophenol and pentachlorophenol on the biota of aquatic systems. Outdoor experiments in compartments of a natural pond. Chemosphere 11: 71-79
Schmidt C, Schnabl H. 1988. Structure-activity-relationship of organic substances and bioindication. Vom Wasser 70: 21-32.
Schultz TW. 1997. Tetratox: Tetrahymena pyriformis population growth impairment endpoint-a surrogate

for fish lethality. Toxicol Method 7: 289-309.
Schultz TW. 1999. Structure-toxicity relationships for benzenes evaluated with tetrahymena pyriformis. Chem Res Toxicol 12: 1262-1267.
Schultz TW, Holcombe GW, Phipps GL. 1986. Relationships of quantitative structure-activity to comparative toxicity of selected phenols in the Pimephales promelas and Tetrahymena pyriformis test systems. Ecotoxicol Environ Saf 12: 146-153.
Schultz TW, Riggin GW. 1985. Predictive correlations for the toxicity of alkyl- and halogen-substituted phenols. Toxicol Lett 25: 47-54.
Schultz TW, Wyatt NL, Lin DT. 1990. Structure-toxicity relationships for nonpolar narcotics: A comparison of data from the Tetrahymena, Photobacterium and Pimephales systems. Bull. Environ. Contam. Toxicol. 44: 67-72.
Schüürmann G, Segner H, Jung K. 1997. Multivariate mode-of-action analysis of acute toxicity of phenols. Aquat Toxicol 38: 277-296.
Sharma HA, Barber JT, Ensley HE, Polito MA. 1997. A comparison of the toxicity and metabolism of phenol and chlorinated phenols by Lemna gibba, with special reference to 2,4,5-trichlorophenol. Environ Toxicol Chem 16: 346-350.
Shigeoka T, Sato Y, Takeda Y, Yoshida K, Yamauchi F. 1988. Acute toxicity of chlorophenols to green algae, Selenastrum capricornutum and Chlorella vulgaris, and quantitative structure-activity relationships. Environ Toxicol Chem 7: 847-854.
Sixt S, Altschuh J. 1997. Prediction of luminescent bacteria toxicity using quantum chemical descriptors: test of a classification scheme. In: Chen F, Schueuermann G, eds. Quant. Struct.-Act. Relat. Environ. Sci.-VII, Proc. QSAR 96. SETAC Press. p. 343-362.
Smith AD, Bharath A, Mallard C, Orr D, Smith K, Sutton JA, Vukmanich J, McCarty LS, Ozburn GW. 1991. The acute and chronic toxicity of ten chlorinated organic compounds to the American flagfish (Jordanella floridae). Arch Environ Contam Toxicol 20: 94-102.
Smith S, Furay VJ, Layiwola PJ, Menezes FJA. 1994. Evaluation of the toxicity and quantitative structure-activity relationships (QSAR) of chlorophenols to the copepodid stage of a marine copepod (Tisbe battagliai) and two species of benthic flatfish, the flounder (Platichthys flesus) and sole (Solea solea). Chemosphere 28: 825-836.
Somasundaram L, Coats JR, Racke KD, Stahr HM. 1990. Application of the Microtox system to assess the toxicity of pesticides and their hydrolysis metabolites. Bull Environ Contam Toxicol 44: 254-259.
Spehar RL. 1986. United states environmental protectiob agency.
Stauber et al., 1994a. In: Warne, MStJ and Westbury, A-M. A compilation of data on the toxicity of chemicals to species in Australasia. Part II: Organic chemicals. Australasian-Journal-of-Ecotoxicology. [print] January, 1999; 5 (1) 21-84. 1999.
Steinberg CEW, Sturm A, Kelbel J, Lee SK, Hertkorn N, Freitag D, Kettrup AA. 1992. Changes of acute toxicity of organic chemicals to Daphnia magna in the presence of dissolved humic material (DHM). Acta Hydroch Hydrobiol 20: 326-332.
Sulaiman AH. 1993. Acute toxicity relationships for two species of fish using a simultaneous testing method. Sci Total Environ 2 : 1001-1009.
Svenson A, Hynning PA. 1997. Increased aquatic toxicity following photolytic conversion of an organochlorine pollutant. Chemosphere 34: 1685-1692.
Svenson A, Zhang L. 1995. Acute aquatic toxicity of protolyzing substances studied as the Microtox effect. Ecotoxicol Environ Saf 30: 283-288.
U.S. Environmental Protection Agency. 1978. In-Depth Studies on Health and Environmental Impacts of Selected Water Pollutants.
Thursby GB, Steele RL, Kane ME. 1985. Effect of organic chemicals on growth and reproduction in the marine red alga Champia parvula. Environ Toxicol Chem 4: 797-805.
Tiensing T, Strachan N, Paton GI. 2002. Evaluation of interactive toxicity of chlorophenols in water and soil using lux-marked biosensors. Journal of Environmental Monitoring 4: 482-489.

Tissot A, Boule P, Lemaire J, Lambert S, Palla JC . 1985. Photochemistry and environment: 10. Evaluation of the toxicity of the phototransformation products of hydroquinone and chlorophenols in aqueous environments. Chemosphere 14: 1221-1230.

Twagilimana L, Bohatier J, Groliere CA, Bonnemoy F, Sargos D. 1998. A new low-cost microbiotest with the protozoan Spirostomum teres: culture conditions and assessment of sensitivity of the ciliate to 14 pure chemicals. Ecotoxicol Environ Saf 41: 231-244.

Veith GD, Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. Environ Toxicol II: 385-391.

Veith GD, DeFoe DL, Bergstedt BV. 1979a. Measuring and estimating the bioconcentration factor of chemicals in fish. J Fish Res Board Can 36: 1040-1048.

Veith GD, Macek KJ, Petrocelli SR, Carroll J. 1979b. An evaluation of using partition coefficients and water solubility to estimate bioconcentration factors for organic chemicals in fish. Journal of the Fisheries Research 36: 1040-1048.

Verschueren K. 1983. Handbook of environmental data on organic chemicals, second edition. New York, USA: Van Nostrand Reinhold Company Inc. 1310 pp.

Virtanen MT, Hattula M-L. 1982. The fate of 2,4,6-trichlorophenol in an aquatic continuous-flow system. Chemosphere 11: 641-649.

Virtanen V, Kukkonen J, Oikari A. 1989. Acute toxicity of organic chemicals to *Daphnia magna* in humic waters. In: Anonymus Nordic symposium on organic environmental chemicals.

Wagner A, Winkler U, Luemmen P. 1989. Mutants of luminous bacteria selected for bioluminescent toxicity tests. J. Biolumin. Chemilumin. 4: 342-345.

Westbury AM. 1998. In: Warne, MStJ and Westbury, A-M. A compilation of data on the toxicity of chemicals to species in Australasia. Part II: Organic chemicals. Australasian-Journal-of-Ecotoxicology. [print] January, 1999; 5 (1) 21-84. 1999.

Wood EM. 1953. 1. The toxicity of 3400 chemicals to fish. Kearneysville, West Virginia: U.S. fish and wildlife service. 196 pp.

Yasuda Y, Tochikubo K, Hachisuka Y, Tomida H, Ikeda K. 1982. Quantitative structure-inhibitory activity relationships of phenols and fatty acids of *Bacillus subtilis* spore germination. J Med Chem 25: 315-320.

Yen JH, Lin KH, Wang YS. 2002. Acute lethal toxicity of environmental pollutants to aquatic organisms. Ecotoxicol Environ Saf 52: 113-116.

Yoshioka Y, Ose Y. 1993. A quantitative structure-activity relationship study and ecotoxicological risk quotient for the protection from chemical pollution. Environ Toxicol Water Qual 8: 87-101.

Yoshioka Y, Ose Y, Sato T. 1985. Testing for the toxicity of chemicals with Tetrahymena pyriformis. Sci Total Environ 43: 149-157.

Yoshioka Y, Ose Y, Sato T. 1986a Correlation of the five test methods to assess chemical toxicity and relation to physical properties. Ecotoxicol Environ Saf 12: 15-21.

Yoshioka Y, Ose Y, Sato T. 1986b. Testing and evaluation of chemical toxicity on Tubifex. Eisei Kagaku 32: 308-311.

RIVM

National Institute
for Public Health
and the Environment

P.O. Box 1
3720 BA Bilthoven
The Netherlands
www.rivm.com