RIVM report 601782003/2007

Environmental risk limits for twelve substances, prioritised on the basis of indicative risk limits

P.L.A. van Vlaardingen, L.R.M. de Poorter,
R.H.L.J. Fleuren, P.J.C.M. Janssen, C.J.A.M.
Posthuma-Doodeman, E.M.J. Verbruggen,
J.H. Vos

Contact:
P. van Vlaardingen
Expert Centre for Substances
E-mail: peter.van.vlaardingen@rivm.nl

This investigation has been performed for the account of the Directorate-General for Environmental Protection, Directorate for Chemicals, Waste and Radiation, in the context of the project 'International and national environmental quality standards for substances in the Netherlands', RIVM-project no. 601782.

National Institute for Public Health and the Environment, PO Box 1, 3720 BA Bilthoven, The Netherlands.
Tel. 31-3—2749111, fax 31-30-2742971

Rapport in het kort

Milieurisicogrenzen voor twaalf stoffen, geprioriteerd op basis van *ad hoc*-MTR waarden

Het RIVM heeft in dit rapport voor twaalf chemische stoffen gedegen milieurisicogrenzen afgeleid. Deze zijn beter onderbouwd dan de tot nu toe gebruikte indicatieve (*ad hoc*) milieurisicogrenzen. Op basis van de milieurisicogrenzen stelt de interdepartementale Stuurgroep Stoffen de milieukwaliteitsnormen vast. De overheid hanteert deze normen bij de uitvoering van het nationale stoffenbeleid en de Europese Kaderrichtlijn Water.

De twaalf chemische stoffen zijn pentabroomdifenylether, para-*tert*-octylfenol, benzo[*b*]-fluorantheen, isodrin, 2-methyl-4,6-dinitrofenol, aniline, epichloorhydrine, 1,2-dibroomethaan, ethinyloestradiol, broommethaan (methylbromide), 4-[dimethylbutylamino]-difenylamine (6PPD) en 3,3'-dichloorbenzidine. Voor deze stoffen zijn tot nu toe alleen indicatieve milieurisicogrenzen afgeleid door het RIZA en het RIVM. De indicatieve waarden van beide instituten verschilden echter vaak meer dan een factor 10. Hierom besloot het ministerie van VROM om voor deze stoffen gedegen milieurisicogrenzen af te laten leiden.

Bij de afleiding van de milieurisicogrenzen gebruikte het RIVM in dit rapport de meest actuele milieuchemische en toxicologische gegevens. De afleiding gebeurde volgens de methode die is voorgeschreven binnen het project (Inter)nationale Normen Stoffen. Dit betekent dat voor water en sediment de methodiek van de Europese Kaderrichtlijn Water is gevolgd. Voor bodem, grondwater en lucht zijn nationale procedures gevolgd, die deels zijn gebaseerd op de technische richtlijn bij de Bestaande Stoffen Verordening.

Er bestaan vier verschillende milieurisicogrenzen: een verwaarloosbaar risiconiveau (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (MTR), het maximaal acceptabele niveau voor water-ecosystemen, specifiek voor kortdurende blootstelling (MAC_{eco}) en een niveau waarbij mogelijk ernstige effecten voor ecosystemen te verwachten zijn (ER_{eco}).

Trefwoorden: milieurisicogrenzen, verwaarloosbaar risiconiveau, maximaal toelaatbaar risiconiveau, ernstig risiconiveau

Abstract

Environmental risk limits for twelve substances, prioritised on the basis of indicative risk limits

The environmental risk limits derived by RIVM for twelve chemical substances, as reported here, are better underpinned than the existing indicative environmental risk limits. Risk limits derived here form the basis for setting environmental quality objectives by the Interdepartmental Steering Committee on Substances. These quality objectives are used by the Dutch government to implement national policy on substances and the European Water Framework Directive.

The twelve chemical substances concerned are pentabromo diphenyl ether, para-*tert*-octylphenol, benzo[*b*]fluoranthene, isodrin, 2-methyl-4,6-dinitrophenol (4,6-dinitro-*ortho*-cresol, DNOC), aniline, epichlorohydrin, 1,2-dibromoethane, ethinylestradiol, methyl bromide, 4-[dimethylbutylamino]diphenylamine (6PPD) and 3,3'-dichlorobenzidine. Only indicative environmental risk limits had been derived for these substances by RIZA and RIVM. However, because these indicative limits differed by at least a factor of 10 for some substances, the Ministry of VROM (Ministry of Housing, Spatial Planning and the Environment) decided to commission a derivation of environmental risk limits for these substances that would be better underpinned.

The derivation was performed according to the methodology prescribed in the project, 'International and national environmental quality standards for substances in the Netherlands'. Up-to-date information on environmental chemistry and toxicology for deriving the environmental risk limits was used. This meant following the methodology of the European Water Framework Directive for water and sediment, and national procedures (partly based on the technical guidance for the Existing Substances Regulation) for soil, groundwater and air.

Four environmental risk limits were distinguished in the derivation: a negligible concentration (NC), a concentration at which no harmful effects are to be expected (MPC), the maximum acceptable concentration for aquatic ecosystems, specifically for short-term exposure (MAC_{eco}), and a concentration at which possible serious effects for ecosystems can be expected (SRC_{eco}).

Key words: environmental risk limits, negligible concentration, maximum permissible concentration, serious risk concentration

Contents

Samenvatting

In dit rapport zijn milieurisicogrenzen afgeleid voor twaalf stoffen. Dit zijn: pentabroomdifenyl-ether (pentaBDE), para-*tert*-octylfenol, benzo[*b*]fluorantheen, isodrin, 2-methyl-4,6-dinitrofenol (4,6-dinitro-*ortho*-cresol, DNOC), aniline, epichloorhydrine, 1,2-dibroomethaan, ethinyloestradiol, broommethaan (methylbromide), 4-[dimethylbutylamino]difenylamine (6PPD) en 3,3'-dichloorbenzidine. Voor de twaalf stoffen was al een *ad hoc*-MTR voorhanden. Een *ad hoc*-MTR is een indicatieve milieurisicogrens, die in korte tijd wordt afgeleid, gebruikmakend van schattingen en/of aannames waar zorgvuldig geëvalueerde gegevens ontbreken. Voor de twaalf behandelde stoffen waren *ad hoc*-MTRs afgeleid door zowel het RIZA als het RIVM. Omdat de verschillen tussen de waarden die door beide instituten waren afgeleid in het algemeen boven een factor 10 lagen, is besloten om voor deze stoffen gedegen MTR af te leiden.
De introductie van de Kaderrichtlijn Water (KRW) in 2000 en de huidige concept-dochterrichtlijn 'Prioritaire Stoffen' bij de KRW hebben een verandering in de normstellingsmethodiek tot gevolg gehad. De herziene normstellingsmethodologie is geïmplementeerd in het raamwerk van het project (Inter)nationale Normen Stoffen (INS). Recent is een RIVM rapport verschenen dat de handleiding voor de herziene normstellingsmethodiek beschrijft (Van Vlaardingen and Verbruggen, 2007). Deze methodiek is voor de normstelling in dit rapport gebruikt. Het grootste verschil in vergelijking met eerdere INS methodiek is dat nu tevens MTR waarden worden afgeleid die de mens beschermen. De KRW normstelling heeft twee MTRs voor water geïntroduceerd. Voor beide geldt dat een bijdrage van een tiende deel van de humaan toxicologische risicogrens van een verbinding wordt toegestaan. Deze methodiek is zonder wijzigingen binnen INS overgenomen. Voor het compartiment bodem is een vergelijkbare methodologie ontwikkeld, en ook voor de andere compartimenten (zeewater, lucht, grondwater) worden MTRs afgeleid op basis van indirecte blootstelling van de mens.
Van de MTR_{water}-waarden afgeleid in dit rapport, zijn er zes lager dan beide *ad hoc*-MTRs. Dit heeft verschillende oorzaken: het gebruik van een lagere humaan toxicologische risicolimiet (pentaBDE), het gebruik van wettelijk bindende normen (epichloorhydrine en dinitro-*ortho*-cresol), limitatie tot een bijdrage aan de humaan toxicologische risicolimiet van maximaal 10% van de route drinkwater-consumptie (1,2-dibroomethaan), nieuwe informatie op het gebied van ecotoxiciteit (ethinyloestradiol) en een strengere berekeningsmethode om visconsumptie te incorporeren in de MTR afleiding (3,3'-dichloorbenzidine). MTR_{water}-waarden voor zes andere stoffen zijn hoger dan één of beide *ad hoc*-MTRs (p-*tert*-octylfenol, benzo[*b*]fluorantheen, isodrin, aniline, methylbromide en 6PPD). Vijf van deze zes MTRs zijn nu gebaseerd op ecotoxicologische gegevens. Het gegeven dat de MTRs afgeleid in dit rapport hoger zijn, is niet eenvoudig te verklaren. Een van de voornaamste oorzaken is dat de afleiding van het *ad hoc*-MTR gebruik maakt van de gecombineerde EUSES/HUMANEX modellen (Bontje *et al.*, 2005). Deze methode gebruikt onder andere een andere waarde voor humane visconsumptie in vergelijking met de KRW methodiek en verscheidene humane blootstellingsroutes terwijl de KRW methodiek alleen visconsumptie en drinkwaterconsumptie in beschouwing neemt. Beide routes zijn in de KRW methodiek gelimiteerd tot een 10% bijdrage aan de totale blootstelling van de mens, terwijl dit in de *ad hoc* methodiek wordt vrijgelaten. Bovendien, omdat de *ad hoc*-MTRs, indicatieve waarden zijn, is hun afleiding minder gedetailleerd gerapporteerd. Deze aspecten belemmeren het verklaren van de verschillen tussen het *ad hoc*- en het gedegen MTR van deze stoffen.
Naast de afleiding van het MTR zijn in dit rapport ook het verwaarloosbaar risiconiveau (VR), het ernstig risiconiveau voor ecosystemen (ER_{eco}) en de maximaal toelaatbare concentratie voor ecosystemen (MAC_{eco}) afgeleid, voor de compartimenten waarvoor dit van toepassing is. Zo wordt bijvoorbeeld het MAC_{eco} alleen voor water afgeleid (geïntroduceerd met de KRW) en wordt het

VR, MTR en ER_{eco} voor sediment alleen afgeleid wanneer de adsorptieconstante zwevend stof-water ($K_{p,\ susp\text{-}water}$) groter is dan 1000.

Summary

In this report, environmental risk limits (ERL) are derived for twelve substances. These twelve substances are: pentabromo diphenyl ether (pentaBDE), para-*tert*-octylphenol, benzo[*b*]fluoranthene, isodrin, 2-methyl-4,6-dinitrophenol (4,6-dinitro-*ortho*-cresol, DNOC), aniline, epichlorohydrin, 1,2-dibromoethane, ethinylestradiol, methyl bromide, 4-[dimethylbutylamino]diphenylamine (6PPD) and 3,3'-dichlorobenzidine. For these substances, two indicative MPCs (maximum permissible concentrations), called *ad hoc*-MPC, for water, derived by two different institutes (RIZA, Institute for inland water management and waste water treatment and RIVM, national institute for public health and the environment), were available. Since differences between *ad hoc*-MPCs by the two institutes were high (generally over a factor of 10) and all of these compounds were prioritised for a thorough ERL derivation, ERL derivation of the twelve compounds was brought together in this report.
The introduction of the Water Framework Directive (WFD) in 2000 and the current draft daughter directive 'Priority Substances' of the WFD has brought about a revised guidance for the derivation of ERLs. This guidance is implemented at the national level in the Netherlands, within the framework of the project (Inter)National Environmental Quality Standards for Substances in the Netherlands (INS). An RIVM report describing this guidance is recently finished and has been used for ERL derivation in the report presented here (Van Vlaardingen and Verbruggen, 2007). The major difference with respect to earlier INS guidance is the inclusion of MPCs that aim at protection of human health. WFD guidance has introduced the derivation of two MPCs for water that each allow for a contribution of one tenth to the human toxicological risk limit for a compound. This methodology is used without further modification. For the compartment soil, a methodology comparable to that in water has been developed, and also for the other compartments (marine water, air, groundwater), ERLs based on indirect exposure of humans.
Of the MPC_{water} values derived in this report, six were lower than both *ad hoc*-MPCs, caused by different reasons: the use of a lower human toxicological risk limit (pentaBDE), the use of legally binding standards (epichlorohydrin and dinitro-*ortho*-cresol), limitation of drinking-water consumption to contribute maximally 10% to the human risk limit (1,2-dibromoethane), increased information on ecotoxicity (ethinylestradiol) and a more stringent calculation method to cover fish consumption in MPC derivation (3,3'-dichlorobenzidine).
MPC_{water} values for the six other substances were higher than one or both of the *ad hoc*-MPC (p-*tert*-octylphenol, benzo[*b*]fluoranthene, isodrin, aniline, methyl bromide and 6PPD). For five of these six substances MPCs have now been derived based on ecotoxicological data. The fact that the MPCs derived in this report are higher, can not be easily explained. One of the main reasons is that derivation of the *ad hoc*-MPC makes use of the combined EUSES/HUMANEX models (Bontje *et al.*, 2005). The *ad hoc* procedure uses e.g. a different human intake rate of fishery products compared to WFD methodology and various human exposure routes are taken into account in HUMANEX, while WFD guidance takes only fish consumption and drinking-water into account, both with a 10% limitation of total human exposure. Moreover, since *ad hoc*-MPCs are indicative values, their derivation is documented with less detail. These aspects hamper an explanation of the differences between the height of the MPCs for the various compounds.
Next to the derivation of the MPC, also the negligible concentration (NC), serious risk concentration for ecosystems (SRC_{eco}) and the maximum acceptable concentration for ecosystems (MAC_{eco}) were derived, for those environmental compartments for which this was applicable. E.g. the MAC_{eco} is only derived for water (the MAC_{eco} is introduced as environmental risk limit by the WFD) and NC, MPC and SRC_{eco} are only derived for sediment when the adsorption constant suspended matter-water ($K_{p,\ susp\text{-}water}$) is higher than 1000.

1. Introduction

1.1 Framework

1.1.1 MPC versus indicative MPC

In the Netherlands, both MPCs (MPC = maximum permissible concentration) and indicative MPCs exist. In Dutch, the indicative MPCs are called *ad hoc*-MPC. The latter term will be used in the text of this report. However, we have replaced *ad hoc*-MPC by 'indicative MPC' in the title of the report since we felt that this would be better understood by readers unfamiliar with the Dutch framework of standard setting.

An *ad hoc*-MPC is derived in a relatively short period of time and only a limited number of databases are screened for physicochemical and toxicological data. The retrieved data are used without careful evaluation. This is different from the derivation of an MPC, for which literature on substance properties and toxicity is searched thoroughly and evaluated carefully, making the resulting standard more reliable. An *ad hoc*-MPC is derived for a substance for which an MPC has not yet been set.
The methodology for *ad hoc*-MPC derivation is laid down in Hansler *et al*. (2006). The methodology for MPC derivation is laid down in Van Vlaardingen and Verbruggen (2007; 2007).

1.2 Description of the underlying project

In this report, environmental risk limits are derived for twelve compounds. All twelve compounds have been prioritised within the framework of the Dutch Emission Guideline for Air ('Nederlandse Emissierichtlijn Lucht', NER) and were placed on the Dutch supplementary priority list ('aanvullende prioritaire stoffenlijst').
The compounds were selected for environmental risk limit (ERL) derivation because two *ad hoc*-MPCs existed for all twelve compounds and the difference between the two *ad hoc*-MPCs was relatively high, i.e. exceeding a factor of 10 in several cases. The main reason that two different *ad hoc*-MPCs can exist for one substance is that the former *ad hoc* value was derived using an older methodology than that currently laid down in Hansler *et al*. (2006).

1.3 Selection of substances

Table 1. Overview of compounds selected for this project.

NL Priority nr.	Compound name as on Dutch priority list	Compound name used in this study	EU-RAR[a]	Type of INS[b] risk limits	WFD[c] priority
GROUP 1					
27	pentabroomdifenylether	pentaBDE	finalised	*ad hoc*	Y
90	para-*tert*-octylphenol	p-*tert*-octylphenol	draft[d]	*ad hoc*	Y
110	benzo[*b*]fluorantheen	benzo[*b*]fluoranthene	draft[e]	*ad hoc*	Y
135	isodrin	isodrin	n.a.[f]	*ad hoc*	N
147	2-methyl-4,6-dinitrofenol	DNOC	n.a.[f]	MPC[h], NC[i]	N
162	aniline	aniline	finalised	*ad hoc*	N
GROUP 2					
56	chloormethoxyoxiraan	epichlorohydrin	n.a.[g]	*ad hoc*	N
57	1,2-dibroomethaan	1,2-dibromoethane	n.a.[g]	*ad hoc*	N
152	ethinylestradiol	ethinylestradiol	n.a.[f]	*ad hoc*	N
172	broommethaan	methyl bromide	n.a.[g]	*ad hoc*	N
192	4-[dimethylbutylamino]difenylamine	6PPD	n.a.[g]	*ad hoc*	N
205	3,3'-dichloorbenzidine	3,3'-dichlorobenzidine	n.a.[g]	*ad hoc*	N

n.a. = not available.
[a]European union-risk assessment report.
[b]INS = International and national environmental quality standards for substances in the Netherlands. In Dutch: (Inter)nationale Normen Stoffen)
[c]WFD = water framework directive.
[d]a *targeted* environmental risk assessment is available.
[e]a draft EU-RAR for coal tar pitch (PCTHT) is available, in which PNECs (predicted no effect concentrations) are derived for individual PAHs (polycyclic aromatic hydrocarbons), amongst which benzo[*b*]fluoranthene.
[f]no IUCLID (international uniform chemical information database) dataset available.
[g]IUCLID dataset available.
[h]MPC = maximum permissible concentration.
[i]NC = negligible concentration.

Table 1 shows the twelve compounds that were selected for this project. Compounds have been assigned to two groups, based on data availability: compounds for which data and/or environmental quality standards (EQSs) have been or are currently being generated in other frameworks (Group 1) and those compounds for which only an *ad hoc* MPC is available (Group 2), see also Chapter 3. The compounds are listed by order of their priority number as given in the Dutch supplementary priority list ('aanvullende prioritaire stoffenlijst'). The order of substances in Table 1 is maintained in all sections throughout this report. Table 1 shows substance name, status in EU-existing substances framework (Council Regulation (EEC) 793/93, column labelled 'EU-RAR'), the status under the Water Framework Directive (WFD; European Parliament and Council Directive 2000/60/EC, column labelled 'WFD priority') and the type of MPC currently available at the Dutch national level (INS framework, INS = (Inter)national environmental quality standards for substances in the Netherlands). For the latter category, there are two possibilities: either an *ad hoc* MPC or an MPC has been derived, as has been outlined in section 1.1.1. Chapter 2 gives detailed information on identification and physico-chemical properties of the selected substances.

1.4 Guidance followed for this project

1.4.1 INS guidance – characteristics of updated guidance

The ERL derivations in this report have in principle been performed using the most recent update of INS guidance (Van Vlaardingen and Verbruggen, 2007). Whether or not a complete ERL derivation is performed according to INS guidance is dependent on possible ongoing compound evaluations in other European regulatory frameworks: existing substances (see section 1.4.3) and the WFD (see section 1.4.4).

The updated INS guidance is in accordance with the guidance by Lepper (2005), which forms part of a draft daughter Directive (COM (2006) 397; EC, 2006a) of the WFD (2000/60/EC; EC, 2000), and the 'Technical Guidance Document (TGD) on Risk Assessment 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 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market' (EC-JRC, 2003). The most important characteristics of the current guidance will be shortly highlighted below.

- WFD guidance applies to the derivation of MPC and consequently NC (negligible concentration), for water, groundwater and sediment. MPC and NC derivation for water and sediment are performed for both the freshwater and marine compartment.
- Guidance for derivation of the MPC for soil follows the EU-TGD.
- Two MPCs based on ecotoxicological data are derived for the water compartment. These are (1) the $MPC_{eco, water}$, which is based on ecotoxicological data and (2) the $MPC_{sp, water}$ (MPC accounting for secondary poisoning), which is derived only in case secondary poisoning in the environment is thought to be of concern.
- WFD guidance introduces two new MPC values for water that are based on a *human toxicological risk limit* (TL_{hh} = threshold limit for human health), which might be an ADI (acceptable daily intake) or TDI (tolerable daily intake), etc. Discerned are (1) the $MPC_{hh\ food, water}$, which is the concentration in water that should protect humans against adverse effects from the substance via fish and other seafood consumption; (2) the $MPC_{dw, water}$ is the concentration in water that should protect humans against adverse effects of the substance by intake of drinking-water. Note that each of these two MPCs are allowed to contribute only 10% to the TL_{hh}. See also section 1.4.2.
- Finally, for the water compartment, the lowest MPC value is selected. It is important to note that MPC and NC derivation now integrates both ecotoxicological data and a human toxicological threshold value. The height of the final environmental risk limit can be determined by either one of these protection objectives.
- WFD guidance departs from the viewpoint that laboratory toxicity tests contain suspended matter in such concentrations, that results based on laboratory tests are comparable to outdoor surface waters. In other words: each outcome of an ERL derivation for water will now result in a <u>total</u> concentration. A recalculation from a dissolved to a total concentration is thus no longer performed within INS framework.
  N.B. This is different from the former Dutch approach, in which each outcome of a laboratory test was considered to represent a *dissolved* concentration. This concentration could then be recalculated to a total concentration using standard characteristics for surface water and suspended matter.

1.4.2 Environmental risk limits protecting humans via indirect exposure

An ERL, as used in the Netherlands, is a concentration in an environmental compartment. The ERL should protect both the ecosystem and humans. Note however, that there are different levels of protection, from negligible risk to serious risk. In this report we also derive environmental risk limits that are aimed at protecting human health, following national (Dutch) guidance. These risk limits will be derived for the environmental compartments: soil, water, groundwater, sediment and air and are expressed as $MPC_{human, comp}$, with 'comp' expressing the environmental compartment for which the risk limit is representing a concentration (e.g. $MPC_{human, water}$ or $MPC_{human, soil}$, etc.). Note that *environmental* risk limits aimed at protecting humans ($MPC_{human, comp}$) should not be confused with *toxicological* risk limits for humans (MPC_{human}). The ERLs derived here are still expressed as a concentration in an environmental compartment, while the MPC_{human} is a standard expressed in mg per kg human bodyweight per day.

With the introduction of the WFD and the technical guidance prepared by the Fraunhofer Institute (FHI) into the INS framework, derivation of ERLs covering human exposure was integrated into the derivation of the MPC. The renewed INS guidance describes this methodology, as well as derivation of $MPC_{human, comp}$ values for the other environmental compartments (Van Vlaardingen and Verbruggen, 2007).

1.4.3 Existing substances

In 1993 the Council of the European Communities adopted Council Regulation (EEC) 793/93 or the 'Existing Substances Regulation' (ESR), thereby introducing a comprehensive framework for the evaluation and control of 'existing' chemical substances. This is a legal instrument that was proposed by European Commission upon approval of the Fourth Community Action Programme on the Environment (1987-1992) by the Council.

The Commission, in consultation with member states has drawn up priority lists for substances that are to be evaluated for both human and environmental risks. For a given prioritised compound, this process has resulted or will result in a European Union Risk Assessment Report (EU RAR) at step 3 of the regulation. In the environmental section of an EU RAR, ecotoxicological environmental risk limits are derived for each environmental compartment, which are called 'predicted no effect concentrations' (PNEC). A PNEC is comparable to the maximum permissible concentration (MPC). For the human-toxicological risk assessment no PNECs are derived for the environmental compartment. Instead of that a human-toxicological threshold value for the daily intake of the substance is used in the risk assessment to evaluate whether or not the combined exposure from several routes exceeds this threshold value. In the updated INS guidance (Van Vlaardingen and Verbruggen, 2007) it is indicated how the data presented in the EU RARs are converted to environmental risk limits for each compartment.

At present the Ministry of Housing, Spatial Planning and the Environment (VROM) has the policy to take over PNEC values from an EU-RAR for an existing substance when these PNECs have already been or are being derived at the time the Ministry seeks advice (that is, requests for an MPC to be derived) for that substance. In principle, an additional literature search is thus not performed.

1.4.4 WFD fact sheets

At present, there is a list of 33 priority hazardous substances for which EQS have been derived, reported in so-called 'Substance Data Sheets'. EQS derivation was performed according to a guidance which is still under development, prepared by the Fraunhofer Institute (Lepper, 2005). Both the guidance and the data sheets are now part of a proposal for a (daughter) Directive (COM (2006) 397; EC, 2006a) amending the WFD (2000/60/EC; EC, 2000). Once adopted, this guidance

and hence the derived EQSs, will be binding for al EU member states. For ERL derivation in the Netherlands, this means that the EQSs for WFD prioritised compounds (as derived in the WFD fact sheets) have to be taken over.

For three compounds subject to this report a WFD fact sheet exists: pentaBDE, p-*tert*-octylphenol and benzo[*b*]fluoranthene. Moreover, EU-RARs are available these compounds: a finalised EU-RAR for pentaBDE, and draft EU-RARs for p-*tert*-octylphenol and benzo[*b*]fluoranthene. The fact sheets for pentaBDE and p-*tert*-octylphenol are based on data from the EU-RARs. For these two compounds, we have closely followed the EQS derivation of the fact sheets. However, for pentaBDE, a modification is proposed, which leads to ERLs that differ than the proposed EQS values of the WFD fact sheets.

In the WFD fact sheet for benzo[*b*]fluoranthene, an *interim* group standard for benzo[*b*]fluoranthene and benzo[*k*]fluoranthene is proposed. In the WFD fact sheet, use of the data in the final EU-RAR on 'coal tar pitch – high temperature fraction' (PCTHT) is proposed, when these data become available. A draft version of the EU-RAR on PCTHT was available for the ERL derivation reported here. Since the EU-RAR is nearly finalised and no changes are expected in the ecotoxicological and human health part of this draft version we have decided to derive ERLs for benzo[*b*]fluoranthene based on this draft EU-RAR.

In the section presenting final ERL proposals (Chapter 9), we will also present the EQS proposals from the WFD fact sheets in a separate table.

2. Substance identification, physico-chemical properties and use

2.1 PentaBDE

2.1.1 Identity

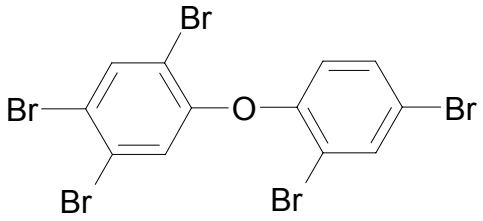

Figure 1. Structural formula of pentaBDE (example component is pentaBDE99 or 2,2',4,4',5-pentabromodiphenyl ether).

Table 2. Identification of pentaBDE.

Parameter	Name or nr.	Source
Chemical name	diphenyl ether, pentabromo derivative	EC, 2001
Common/trivial/other name	pentaBDE	EC, 2001
CAS nr.	32534-81-9	EC, 2001
EC nr.	251-084-2	
SMILES code	Brc1cc(c(cc1Oc2c(cc(cc2)Br)Br)Br)Br	
INS priority nr.	27	

Commercially available pentabromo diphenyl ether (pentaBDE) is not a pure substance but is a mixture of congeners. The name pentabromo diphenyl ether denotes the main component of the mixture. The actual composition of commercially available pentaBDE varies between manufacturers, but in the EU-RAR information available for one mix was found to be comparable to all mixes. DE-71, Bromkal 70 and Satyex 115 were found to be representative commercial mixes of pentaBDE, although details of the percentage content of the different isomers are not available. The commercial products Bromkal 70 and Saytex 115 are no longer in production or supplied to the EU.
Generally, the mixes of PBDE contain pentaBDE (CAS 32534-81-9, 50-62% w/w) and tetrabromo diphenyl ether (CAS 40088-47-9, 24-38% w/w). Additionally, each group of congeners will exhibit a number of isomeric forms, although it is not clear which, or in what proportion, and whether this will alter depending on the supplier/manufacturing process. Impurities comprise, where stated, some or all of the following: tribromo diphenyl ether (CAS 49690-94-0, 0-1% w/w), hexabromo diphenyl ether (CAS 36483-60-0, 4-12% w/w), heptabromo diphenyl ether (CAS 68928-80-3, trace).
Source: EC (2001).

2.1.2 Physico-chemical properties

Physico-chemical properties are shown in Table 3. Bold values indicate values used in calculations. The choices for these selections were made in the EU-RAR and the WFD datasheet for pentaBDE.

Table 3. Selected physico-chemical properties of pentaBDE. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	564.69	70.8% bromine by weight	EC, 2001
Water solubility	[mg.L^{-1}]	0.0133	commercial product with	EC, 2001
		0.0024	for pentaBDEs and	EC, 2001
		0.0109	for tetraBDEs	EC, 2001
		7.86×10^{-5}	at 25ºC; estimated from log K_{ow}[a]	US EPA, 2004
		0.0107	estimated using fragment method	US EPA, 2004
pK_a	[-]	n.a.	does not dissociate	
log K_{ow}	[-]	**6.57**	generator column method; 25ºC[b]	EC, 2001
		7.88	calculated[c]	EC, 2001
		6.46 – 6.97	measured; HPLC method	EC, 2001
log K_{oc}	[-]	5.42	QSAR[f] for predominantly hydrophobics (TGD) using log K_{ow} = 6.57	Anonymus, 2004; EC, 2001
		5.33-**5.75**	QSAR for predominantly hydrophobics (TGD) using log K_{ow} range of 6.46 – 6.97	Anonymus, 2004; EC, 2001
Vapour pressure	[Pa]	$\mathbf{4.69\times10^{-5}}$	at 21ºC; determined with spinning rotor gauge	EC, 2001
		$3.3\text{x}10^{-6}$	at 25ºC; modified Grain method	EC, 2001
		$2.9\text{-}7.3\text{x}10^{-5}$	at 25ºC; GC technique	EC, 2001
Melting point	[°C]	-7 - -3[d]		EC, 2001
Boiling point	[°C]	n.r.	decomposes at >200ºC (commercial product)[e]	EC, 2001
Henry's law constant	[Pa.m^3.mol^{-1}]	0.12	at 25ºC bond method	US EPA, 2004
		0.36	at 25ºC group method	US EPA, 2004
		23.4	at 25ºC P_v/S_w estimate EPI Suite	US EPA, 2004

n.r. = not reported, n.a. = not applicable.
[a]Estimated from log K_{ow}, with log K_{ow} = 7.66. No melting point equation used.
[b]The study of MacGregor and Nixon (1997) is elaborated upon in the EU-RAR of pentaBDE. This log K_{ow} is used for the risk assessment.
[c]EU-RAR reports that theoretical basis for the calculated value or the original evidence have not been evaluated.
[d]Original reports have not been submitted. Therefore, validity of data could not be checked.
[e]The EU-RAR reports that no boiling point is available, but that it decomposes in the temperature range 200-300ºC. Moreover, since the commercial substance is a mixture, the EU-RAR postulates that pentaBDEs are expected to exhibit a wide temperature range for decomposition. This particular physico-chemical parameter is found not really applicable to this type of substance (WHO, 1994).
[f]QSAR = quantitative structure activity relationship.

It should be noticed that log K_{ow} values for individual PBDE congeners 47, 85, 99, 100, 153, and 154 (tetra- to hexaBDEs), which can be found in commercial pentabromo diphenyl ether, determined with the slow-stirring method range from 6.81 to 7.90 (Braekevelt *et al.*, 2003). This is considerably higher than the value determined for the commercial mixture of 6.57. In this study the tribromo diphenyl ether congeners 17 and 28 had lower log K_{ow} values of 5.74 and 5.94. Similarly, the vapour pressure of individual congeners 47, 99, 85, and 138 (tetra- to hexaBDEs), determined with the gas chromatographic method, range from 2.19×10^{-5} to 1.51×10^{-6} Pa (Tittlemier and Tomy, 2001), which is lower than the value determined for the commercial mixture of 4.69×10^{-6} Pa. The tribromo diphenyl ether congener 28 had a higher vapour pressure of 1.77×10^{-4} Pa. Thus, it seems that with the methods used for the studies selected in the EU RAR the values for these parameters are strongly influenced by the small amount of tribromo diphenyl ether congeners.

2.1.3 Behaviour

Information on behaviour of pentaBDE is cited from the EU-RAR for pentaBDE (EC, 2001).

'PentaBDE may volatize or leach from polymer matrixes during the lifetime of an article. Losses of foam particles containing the substance may also occur. However, pentaBDE has a very low vapour pressure, and, therefore, losses from polyurethane foam due to volatilisation is expected to be low. Given that the major use of pentaBDE is in foam for furniture, seating and automobile use, leaching potential from the foam is expected to be low, because it is unlikely that the foam cushioning will be washed.

Release of particulate waste from weathering, wear, etc., during the service life of the product is also expected to be low. Release to the environment could occur at the end of the articles' services life during disposal operations. It is probable that most polyurethane foam for furniture use ends up in landfills or incineration installations. The amount of pentaBDE disposed of each year is estimated to be 1,036 tonnes/year in the whole EU. An overview of estimated releases of pentaBDE from various sources, can be found in the RAR for pentaBDE.' (EC, 2001)

2.1.4 Use

Information on use of pentaBDE is cited from the EU-RAR for pentaBDE (EC, 2001).

'Production of pentaBDE ceased in the EU in 1997. The annual world-wide production of all polybrominated diphenyl ethers was approximately 40,000 tonnes/year, which was broken down as: 30,000 tonnes of decabromo diphenyl ether, 6,000 tonnes of octabromo diphenyl ether and 4,000 tonnes of pentabromo diphenyl ether. These global figures were published in 1994, but the EU-RAR did not report for which year these data were reported.
The combined import and production figure for the EU of all polybrominated diphenyl ethers was 11,000 tonnes/year in 1989. Assuming that pentaBDE accounts for 10% of the total EU usage of polybrominated diphenyl ethers, it can be estimated that around 1,100 tonnes of pentaBDE are used each year in the EU. In the Netherlands, around 350 tonnes/year of pentaBDE were thought to be used as a flame retardant. The level of use of pentaBDE in the EU at the time of creation of the RAR of pentaBDEs was determined to be around 100-125 tonnes/year, with a similar amount being estimated to be imported into the EU in finished goods. PentaBDE was produced in the EU by the direct bromination of diphenyl ether using a Friedel-Crafts catalyst.

PentaBDE is a flame retardant of the additive type, meaning that it is physically combined with the material being treated instead of chemically combined. This has as consequence that the flame retardant may diffuse out of the treated material to some extent. The amount of flame retardant used depends on a number of factors, but typically the flame retardants are added at concentrations between 5 and 30% by weight.
The production of pentaBDE was ceased in the EU in 1997. No data are available for emission from polyurethane foam production. Major use of pentaBDE appears to be as a flame retardant additive in flexible polyurethane foam for furniture and upholstery. Other reported uses are flame retardant additive in epoxy resins, in phenolic resins, in unsaturated polyesters and in textiles.' (EC, 2001)

2.2 p-*tert*-octylphenol

N.B. Data for p-*tert*-octylphenol in this report are cited from Anonymus (2005a) and Brooke *et al*. (2005). Some physicochemical data were added for comparison.

2.2.1 Identity

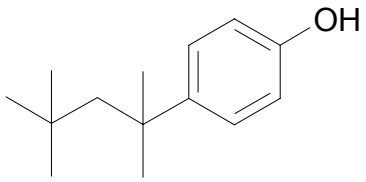

Figure 2. Structural formula of p-tert-octylphenol.

Table 4. Identification of p-tert-octylphenol.

Parameter	Name or nr.	Source
Chemical name	4-tert(iary)-octylphenol (IUPAC[a])	Brooke *et al.*, 2005
Common/trivial/other name	octylphenol, p-*tert*-octylphenol, 4-(1,1,3,3-Tetramethylbutyl)phenol (EINECS), p-(1,1,3,3-tetramethylbutyl)phenol	Brooke *et al.*, 2005
CAS nr.	140-66-9	Brooke *et al.*, 2005
EC nr.	205-426-2	Brooke *et al.*, 2005
SMILES code	Oc(ccc(c1)C(CC(C)(C)C)(C)C)c1	Brooke *et al.*, 2005
INS priority nr.	90	

[a]International union of pure and applied chemistry.

The data presented in this section and the data used for ERL derivation relate to the structure presented above (Figure 2). The presented molecule is the only isomer currently available commercially in Europe. However, it should be noted that iso-octylphenol (Figure 3; CAS nr. 11081-15-5) is also considered to be a high production volume chemical by the European Chemicals Bureau (ECB), and it has been prioritised by OSPAR (Oslo-Paris convention), although it is no longer used commercially. Other different para-octylphenol isomers exist, but Brooke *et al*. (2005) state that marketing of these substances in Europe has ceased.

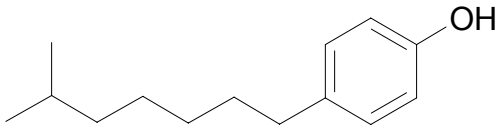

Figure 3. Structural formula of iso-octylphenol, CAS no. 11081-15-5.

2.2.2 Physico-chemical properties

Table 5. Physico-chemical properties of p-tert-octylphenol. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[$g.mol^{-1}$]	206.33		Brooke *et al.*, 2005
Water solubility	[$mg.L^{-1}$]	5	25°C	Anonymus (2005a)
		12.6	20.5°C	Anonymus (2005a)
		19		Brooke *et al.*, 2005
		32	Calculated (fragment method)	US EPA, 2004
		5.6	Calculated (from log K_{ow} : 5.28)	US EPA, 2004
pK_a	[-]	10.33	at 25°C	Brooke *et al.*, 2005
log K_{ow}	[-]	3.96		Anonymus (2005a)
		4.12	OECD[a] shake flask	Brooke *et al.*, 2005
		4.5		Anonymus (2005a)
		5.3		Anonymus (2005a)
		5.28	calculated	US EPA, 2004
		5.16	calculated	BioByte, 2006
log K_{oc}	[-]	**3.43**	estimated from log K_{ow}	Brooke *et al.*, 2005
		4.3		Anonymus (2005a)
		4.19	calculated	US EPA, 2004
Vapour pressure	[Pa]	0.064		Anonymus (2005a)
		0.21		Brooke *et al.*, 2005
		0.076	calculated (modified Grain method; melting point used)	US EPA, 2004
Melting point	[°C]	80.5	mean of available range	Brooke *et al.*, 2005
Boiling point	[°C]	281.5	mean of available values and ranges	Brooke *et al.*, 2005
Henry's law constant	[$Pa.m^3.mol^{-1}$]	**0.52**	measured, 25°C	Brooke *et al.*, 2005
		0.699	20°C	Anonymus (2005a)
		0.456	calculated (bond contribution method)	US EPA, 2004
		0.698	calculated (group contribution method)	US EPA, 2004

[a]Organisation for economic co-operation and development.

2.2.3 Behaviour

All information in this section is cited from Brooke *et al*. (2005).
Based on the Henry's law constant of 0.52 $Pa.m^3.mol^{-1}$, a $K_{air\text{-}water}$ of 2.1×10^{-4} $m^3.m^{-3}$ is calculated, indicating that volatilisation of p-*tert*-octylphenol from water is negligible. Atmospheric degradation will occur rapidly by hydroxyl radicals, a half-life of 0.25 days is estimated under assumption of 12 hours daylight and 1.5×10^6 $radicals.cm^{-3}$. Hydrolysis is thought to be of minor importance, although not supported by experimental evidence. Photolysis might play a role as an abiotic degradation route although experimental evidence is lacking and this degradation route is not further detailed.

p-*tert*-Octylphenol is not readily biodegradable. Degradation in river water microcosms was observed, with half-life values of 7 to 50 days. A study with seawater showed a half-life of 30-60 days. In an experiment with anaerobically incubated sediments no degradation was observed. Aerobically incubated marine sediments revealed complete removal of p-*tert*-octylphenol after 70 days, while no degradation occurred under anaerobic conditions. No experimental data on degradation of p-*tert*-octylphenol in soil were retrieved.
Few experimental data on adsorption are discussed. Results from batch adsorption studies with river sediment showed K_d values of 6000 - 7000 $L.kg^{-1}$, with K_{oc} values of 3500 – 18000 $L.kg^{-1}$.

2.2.4 Use

The use of p-*tert*-octylphenol in Europe in 2001 consisted for 98% of production of phenol-formaldehyde resins ('phenolic resins' also known as Bakelite) and for the remaining 2% of the production of octylphenol ethoxylates and derivatives. The phenolic resins produced using p-*tert*-octylphenol are further processed in:
- rubber compounding for tyres (accounting for up to 98% of total use);
- electrical insulating varnishes;
- printing inks;
- ethoxylated resins;
- minor uses like resins in foundry industry and paints used in marine applications.

The use of octylphenol ethoxylates is of less quantitative importance compared to phenolic resins. Main uses of ethoxylated octylphenols are: emulsion polymerisation, textile and leather auxiliaries, formulations of pesticides and veterinary medicines, water-based paints and production of octylphenol ether sulphates. Many minor uses of ethoxylates are also known, individual uses are generally fractions of tonnes (on a yearly basis).

2.2.5 Endocrine disruptive properties

p-*tert*-Octylphenol may elicit endocrine mediated responses. Because of its structural similarity with natural hormones, p-*tert*-octylphenol has affinity for certain hormone receptor sites and may therefore interfere and/or compete with the role of the endogenous hormones (hormone mimicking effects). p-*tert*-Octylphenol is able to bind to the estrogen receptor but it is also able to displace androgen from the androgen-receptor.
There are other possible modes of action that may lead to interference with the endocrine system, together termed non receptor mediated endocrine disruption. The latter type of effects are identified at the 'biochemical level', an example of which is disruption of cytochrome P450 enzymes, which effects steroid genesis, which may eventually lead to effects on the endocrine system. The above text is based on Anonymus (2005a).

Brooke *et al*. (2005) give an extensive overview of studies with p-*tert*-octylphenol that have focused on endocrine related effects in various organisms (amphibians, fish, crustaceans, molluscs)

and test systems, both *in vivo* and *in vitro*. We subscribe their point of view on the hierarchy of relevance of test methods to measure endocrine-mediated responses, which was adopted from the OECD. Longer term *in vivo* studies considering effects on reproduction and/or development are more important than short term *in vivo* studies, which are generally of greater relevance than *in vitro* assays.
Brooke *et al*. have also focused on 'relevant endpoints for the detection of population-community effects' in line with a CSTEE (scientific committee on toxicity, ecotoxicity and the environment) opinion (CSTEE, 1999). This point of view corresponds with the strategy that has been followed within the INS framework. In short: only studies that show endocrine mediated effects to be related to endpoints that might result in effects at the population level (e.g. reproduction, mortality, growth, teratogenicity) for the test species considered, are relevant for direct use in ERL derivation. Studies resulting in other endpoints: biochemical parameters such as vitellogenin levels, changes in gonadosomatic index, or histopathological changes, etc., of which the direct relevance at the population level is not clear, are considered, but not primarily used for ERL derivation. These two types of studies are assessed separately. Only if the evidence from the latter type of studies is strong enough to support the hypothesis that the ERL derived on the basis of 'classical' endpoints is *not protective* for effects at the population level induced by endocrine mediated effects, is an adjustment of the ERL reconsidered.

2.3 Benzo[*b*]fluoranthene

2.3.1 Identity

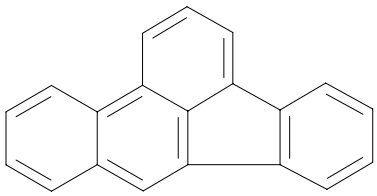

Figure 4. Structural formula of benzo[b]fluoranthene.

Benzo[*b*]fluoranthene belongs to the class of compounds called 'polycyclic aromatic hydrocarbons' or 'polynuclear aromatic hydrocarbons' (PAH). The compounds generally designated as PAH consist entirely of carbon and hydrogen and do not possess substituted groups. PAHs are relatively stable compounds, although they can be degraded and metabolised. Carbon atoms are structured into rings of six (sometimes five) atoms and these rings are fused by sharing one carbon-carbon bond. PAH molecules are flat, i.e. all carbon and attached hydrogen atoms lie in the same plane. The double bonds between carbon atoms as drawn in the molecular structure bring about the presence of π-electrons that are located in orbits above and below the molecule, but in the same plane. The nature of an aromatic system is that is possesses resonance structures, meaning that the π-electrons have the possibility to freely move from one carbon-carbon bond to the next, while the molecule remains its integrity.

Table 6. Identification of benzo[b]fluoranthene.

Parameter	Name or nr.	Source
Chemical name	benzo[*b*]fluoranthene	
Common/trivial/other name	benzo(*e*)acephenanthrylene, 3,4-Benz(*e*)acephenanthrylene, 2,3-Benzfluoranthene, 3,4-Benzfluoranthene, 2,3-Benzofluoranthene, 3,4-Benzofluoranthene, I Benzo(*e*)fluoranthene, B(*b*)F	ECB, 2005, IARC, 1983
CAS nr.	205-99-2	EC, 2006b
EC nr.	205-911-9	ECB, 2005
SMILES code	c12ccccc1cc3c4ccccc4c5c3c2ccc5	
INS priority nr.	110	

2.3.2 Physico-chemical properties

Table 7. Physico-chemical properties of benzo[b]fluoranthene. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	252.32		Anonymus, 2005c
Water solubility	[mg.L^{-1}]	**0.00128**	Generator column method	EC, 2006b
		0.00109	Generator column method	De Maagd *et al*., 1998
		0.0015	Generator column method	Wise *et al*., 1981
		0.0020	Fragment method	US EPA, 2004
		0.013	Calculated from log K_{ow} and Mp	US EPA, 2004
pK_a	[-]	n.a.		EC, 2006b
log K_{ow}	[-]	**6.12**		BioByte, 2006
		6.11	Fragment method	US EPA, 2004
log K_{oc}	[-]	**5.91**	Karickhoff equation and log K_{ow} = 6.12	EC, 2006b
Vapour pressure	[Pa]	**3.3x10^{-6}**	25°C; estimated using EPIWIN	EC, 2006b
Melting point	[°C]	168.3		EC, 2006b
Boiling point	[°C]	481		EC, 2006b
Henry's law constant	[Pa.m^3.mol^{-1}]	**0.051**	20°C; method: gas stripping	Ten Hulscher *et al.*, 1992; EC, 2006b
		0.082	Bond contribution method	US EPA, 2004
		0.021	Group contribution method	US EPA, 2004

n.a. = not applicable.

2.3.3 Behaviour

The text in this section is cited from EC (EC, 2006b).
'PAH are chemically stable, with no functional groups that results in hydrolysis. Under environmental conditions, therefore, hydrolysis does not contribute to the degradation of PAH. The main abiotic transformation is photochemical decomposition, which in natural water takes place only in the upper few centimetres of the aqueous phase. The results from standard tests for biodegradation in water show that PAH with up to four aromatic rings are biodegradable under aerobic conditions but that the biodegradation rate of PAH with more aromatic rings is very low. Although the biodegradation pathway of the different PAHs is very similar their biodegradation rates differ considerably. In general the biodegradation rate decreases with increasing number of aromatic rings.
Biodegradation is the major mechanism for removal of PAH from soil, although PAHs with fewer than four aromatic rings may also be removed by volatilization and photolysis. Many different species of bacteria (both Gram-negative and Gram-positive), fungi, yeasts and algae are known to degrade PAHs of which bacteria are generally assumed to be the most important group of soil micro-organisms contributing in the biodegradation of PAHs in soils. Fungi may play a significant role in PAH degradation in the top soil.
Like for the aquatic environment, there is a relationship between PAH environmental persistence and increasing number of benzene rings which is consistent with the results of various studies correlating environmental biodegradation rates and PAH molecule size, probably due to changes in the aqueous solubility, bioavailability and structural stability of PAHs through the compound group.

For a five ring PAH like benzo[*b*]fluoranthene, a range of half-life values of 45-125 days is given.'

2.3.4 Use

PAHs originate from fossil fuels, like crude oil and coal. They are re-emitted into the environment by both biogenic and anthropogenic processes using these resources, in all versatility: vulcano-eruptions, forest fires, extraction of oil and oil refining industry, wood preservation, smoking of cigarettes, exhaust fume of petrol engines, etc.. PAH can also be formed during incomplete combustion of organic material (wood, fuel), via pyrolysis and pyrosynthesis. PAHs are used as intermediates in production of plastics, plasticisers, pigments, dyes, pesticides, etc.

2.3.5 Carcinogenicity

Benzo[*b*]fluoranthene is genotoxic. Exposure of rats to benzo[*b*]fluoranthene by lung implantation resulted in tumour formation, as did intraperitoneal exposure of newborn mice. Skin painting and initiation/promotion studies in mice were positive. DNA adducts were detected *in vitro* and *in vivo*. (WHO, 1998)

BbF is a potential human carcinogen, it is categorised as a class 2B carcinogen in the International Agency for Research on Cancer (IARC) monograph (IARC, 1983).

2.4 Isodrin

2.4.1 Identity

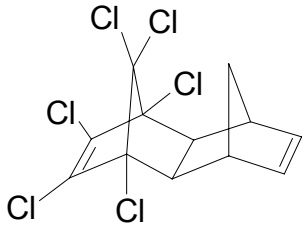

Figure 5. Structural formula of isodrin (source: ECB, 2005).

Table 8. Identification of isodrin.

Parameter	Name or nr.	Source
Chemical name	(1α,4α,4aβ,5β,8β8aβ)-1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene	ECB, 2005
Common/trivial/other name	isodrin	
CAS nr.	465-73-6	
EC nr.	207-366-2	ECB, 2005
SMILES code	C(=C(C(C1(Cl)Cl)(C(C(C=CC23)C2)C34)Cl)Cl)(C14Cl)Cl	
INS priority nr.	135	

2.4.2 Physico-chemical properties

EPI Suite (US EPA, 2004) returns a match on CAS nr. for isodrin and generates estimated values for physico-chemical parameters for isodrin. Bioloom (BioByte, 2006) does not contain data on isodrin upon CAS nr. entry. The smiles code for isodrin is equal to that of its stereoisomer aldrin. Therefore, upon entry of the SMILES code for isodrin, Bioloom returns physico-chemical parameter estimates for aldrin. Since aldrin and isodrin are structurally closely related, it was

decided to tabulate log K_{ow} and log K_{oc} estimates for aldrin in Table 9 (values for aldrin are marked with a * symbol).

Table 9. Physico-chemical properties of isodrin. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	364.92		MDL Information Systems, 1997
Water solubility	[mg.L^{-1}]	8.67×10^{-3}	Calculated; for 25°C; from log K_{ow}=4.68	US EPA, 2004
		2.40×10^{-3}	Calculated fragment method	US EPA, 2004
		1.42×10^{-2}	Calculated	Anonymus, 2005c
pK_a	[-]	n.a.		
log K_{ow}	[-]			
		3.01*	Considered unreliable (Bioloom)	BioByte, 2006
		5.52*	unknown	Garten and Trabalka, 1983
		5.66*	Shake flask	Geyer *et al.*, 1984
		5.74*	Measured; HPLC method	Finizio *et al.*, 1997
		6.50*	Measured, slow stirring	BioByte, 2006, De Bruijn *et al.*, 1989
		6.75	Calculated; KOWWIN v1.67	US EPA, 2004
		7.40*	Determined using TLC	Briggs, 1981
log K_{oc}	[-]	5.02	Calculated, PCKOCWIN v1.66	US EPA, 2004
		4.68*	Recalculated from exp. log K_{om}	Briggs, 1981
Vapour pressure	[Pa]	5.89×10^{-3}	Calculated, at 25°C; MPBPWIN v1.41	US EPA, 2004
Melting point	[°C]	120.88	Calculated; MPBPWIN v1.41	US EPA, 2004
		240		Anonymus, 2005c
Boiling point	[°C]	329.86	Calculated; MPBPWIN v1.41	US EPA, 2004
Henry's law constant	[Pa.m^3.mol^{-1}]	39.2	Calculated; Henrywin v3.10	US EPA, 2004
		247	Calculated; P_v/S_w	US EPA, 2004

n.a. = not applicable.
* = value determined for aldrin.

2.4.3 Use

Isodrin is not and has not been registered in authorised plant protection products in the Netherlands (CTB, 2005a).

2.5 DNOC

2.5.1 Identity

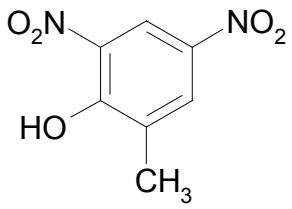

Figure 6. Structural formula of DNOC.

Table 10. Identification of DNOC.

Parameter	Name or nr.	Source
Chemical name	2-methyl-4,6-dinitrophenol	ECB, 2005
Common/trivial/other name	4,6-dinitro-*o*-cresol, DNOC	ECB, 2005
CAS nr.	534-52-1	
EC nr.	208-601-1	ECB, 2005
SMILES code	O=N(=O)c(cc(N(=O)=O)c(O)c1C)c1	
INS priority nr.	147	

2.5.2 Physico-chemical properties

Table 11. Physico-chemical properties of DNOC. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	198.14		US EPA, 2004
Water solubility	[mg.L^{-1}]	130[a]	>99%; at 15°C	Luttik and Linders, 1990
		198[a]	20°C;experimental	Anonymus, 2005c
pK_a	[-]	4.31	21°C, experimental	BioByte, 2006
		4.48	20°C	Tomlin, 2002
log K_{ow}	[-]	**2.13**	Measured (MlogP)	BioByte, 2006; Physprop
		2.39		Luttik and Linders, 1990
log K_{oc}	[-]	2.77[b]	adsorbent is solids from municipal wastewater plant, % o.c. not reported	Dobbs *et al.*, 1989
		1.54	sand soil; pH 4.4; 3.3% o.m.; $^1/_n$ = 1.33; uncorrected for pH	Luttik and Linders, 1990
		1.97	peat soil; pH 5.5; 25.7% o.m.; $^1/_n$ = 1.04; uncorrected for pH	Luttik and Linders, 1990
		1.95 – 2.80	see Table 12	Jafvert, 1990
		2.57[c]	muck soil; K_d at pH 3.0; 49.5% o.c.; uncorrected for pH	Sheng *et al.*, 2001
		2.78	Calculated	US EPA, 2004
Vapour pressure	[Pa]	8.65x10^{-3} [d]	25°C	Luttik and Linders, 1990
		6.92x10^{-3} [d]	25°C	Luttik and Linders, 1990
Melting point	[°C]	**86**		Luttik and Linders, 1990
Boiling point	[°C]	**312**		Luttik and Linders, 1990
Henry's law constant	[Pa.m^3.mol^{-1}]	**5.66x10^{-3}**	at 20°C; calculated from experimental S_w and P_v from Luttik and Linders (1990)	this report

n.r. = not reported, n.a. = not applicable.
[a]Selected value is **176.6** mg.L^{-1}, which is the geometric mean of 130 mg.L^{-1} at 15°C and 198 mg.L^{-1} at 20°C, after recalculation to 20°C using the Arrhenius equation (E_a of 2.7×10^4 J.mol^{-1}).
[b]Because of the nature of the adsorbent and the missing value for organic carbon content, this K_{oc} value is deemed less useful.
[c]Sorption was well described by a Langmuir sorption isotherm, with a K_L of 1700 L.mmol^{-1}. In the linear part of the isotherm, up to concentrations of approx 0.1 µM (~20 µg.L^{-1}) aqueous and < 100 µmol.kg^{-1} (sorbed), log K_d was determined to be 4.24 for the homo ionic Cs^+ kaolinite clay.
[d]Selected value is 7.74x10^{-3} Pa, is geometric mean of the two listed values.

2.5.3 Behaviour

DNOC is used as an insecticide, herbicide and acaricide. Its mode of action is uncoupling of oxidative phosphorylation, leading to membrane disruption. DNOC is a weak phenolic acid, which occurs in the ionised form in most natural Dutch surface waters (pH 7 or higher), in view of its pK_a of 4.3 to 4.5. In more acidic conditions, such as in certain groundwater areas, the proportion of neutral DNOC increases. Its tendency to evaporate from water is low, regarding the estimated Henry coefficient of 5.7×10^{-3} Pa.m^3.mol^{-1}.

Adsorption of DNOC type compounds (acidic nitro aromatics) to natural soils and sediments is governed by both the clay and organic matter fraction as well as the pH. The extent of sorption to both adsorbent types is determined by different factors. For clay, the type of clay mineral, its surface charge and the type of hydrated cations covering the clay surfaces, are important parameters, while sorption on organic matter is dominated by hydrophobic interactions (E.g. Sheng *et al.*, 2001; Haderlein *et al.*, 1996; Weissmahr *et al.*, 1997). A very clear influence of pH on the

sorption of DNOC on homo-ionic Cs^+-kaolinite was demonstrated by Haderlein and Schwarzenbach (1993). K_d as a function of pH could be very well described by plotting the neutral fraction of DNOC. Kd was maximally 18000 $L.kg^{-1}$ (at an aqueous concentration of 20 $\mu g.L^{-1}$). Haderlein *et al*., (1996) report a Kd for DNOC of 37000 on a homo-ionic K^+-montmorillonite. Note that a clay (not a soil) was used in these studies and that the clay was prepared as homo-ionic, with only one cation, Cs^+ or K^+, both of which have a relatively high free energy of hydration, i.e. the ion is easily replaced at cation exchange sites. Both studies showed that sorption on the minerals (kaolinite and montmorillonite) is dramatically decreased when other cations are used (e.g. Ca_2^+, Na^+, Mg^{2+}). In a study in which adsorption isotherms at various pH were measured using samples from a sandy aquifer, Broholm *et al*. (2001) could also relate DNOC sorption to pH by plotting the neutral DNOC fraction versus K_d. K_d reached a maximum value of approximately 14 $L.kg^{-1}$. The aquifer was low in organic matter content (0.007-0.015%) and the extent of sorption could not be explained by hydrophobic sorption to organic matter. Although the mechanism of sorption was not elucidated in this study, clay was believed to be the major adsorbent. Sheng *et al*. (2001) also showed that DNOC sorption to a K^+ (an easily replaced hydrated cation) saturated smectite clay (not a soil) was much higher than sorption to a muck soil containing 49.5% organic carbon. The K_d values, determined at pH 3, were 2490 and 184, for K^+-smectite and muck soil, respectively. Correction of DNOC sorption for the neutral fraction does not explain variation satisfactorily when applied to the data of Jafvert (1990), as illustrated by the values of K_d^{HA} in Table 12 (results from one sediment were omitted because of 'negative adsorption'). In this study, K_d values determined from sorption isotherms on 13 natural soils and sediments are reported. The correction for the neutral fraction was performed using the following equations (Haderlein and Schwarzenbach, 1993):

$$K_d = \alpha_0 K_d^{HA}$$

$$\alpha_0 = \frac{1}{1+10^{(\mathrm{pH}-\mathrm{p}K_a)}}$$

The mean of K_d^{HA} values is 3781, with a standard deviation of 4162, i.e. a variation coefficient of 330%. Correction of sorption for the neutral fraction for the more acidic sediments (nr. 14 and 24) is especially poor: sorption in these sediments is higher than in non-acidic soils, as reflected by higher K_p values, but this cannot be explained by assuming that only the neutral fraction contributes to sorption. This illustrates that in these natural soils, the effect of pH alone can not explain sorption behaviour, in contrast to the studies where homo-ionic clays or aquifer material low in organic matter content where used (Haderlein and Schwarzenbach, 1993; Broholm *et al.*, 2001).

Table 12. Sorption of DNOC on natural soils and sediments: K_d values, correction to neutral DNOC fraction and recalculation to K_{oc} values.

Sediment	% o.c.	pH	K_p	α_0 (=$f_{neutral}$)	K_d^{HA}	K_{oc}	log K_{oc}	Reference
5	2.28	7.15	4.02	0.0014	2785	176	2.25	Jafvert, 1990
8	0.15	8.29	0.38	0.00010	3629	253	2.40	Jafvert, 1990
11	1.50	7.92	3.57	0.00025	14547	238	2.38	Jafvert, 1990
12	2.33	7.53	5.18	0.00060	8602	222	2.35	Jafvert, 1990
13	3.04	7.00	4.75	0.0020	2331	156	2.19	Jafvert, 1990
14	0.48	4.27	2.89	0.52	6	602	2.78	Jafvert, 1990
15	0.95	7.27	2.35	0.0011	2146	247	2.39	Jafvert, 1990
16	1.20	7.47	1.19	0.00069	1721	99	2.00	Jafvert, 1990
18	0.66	7.52	1.05	0.00062	1704	159	2.20	Jafvert, 1990
22	1.67	7.53	3.62	0.00060	6011	217	2.34	Jafvert, 1990
24	0.95	4.47	5.93	0.41	15	624	2.80	Jafvert, 1990
25	0.76	7.75	0.68	0.00036	1874	89	1.95	Jafvert, 1990
-	49.5	3.0	184	0.95	193	372	2.57	Sheng *et al.*, 2001
-	3.3	4.4	34.7	0.45	77	1051	3.02	Luttik and Linders, 1990
-	25.7	5.5	93	0.061	1539	363	2.56	Luttik and Linders, 1990

Although the discussion above makes clear that normalisation of K_d values to soil or sediment organic carbon content disregards other sorption mechanisms for DNOC, it does explain sorption in the less acidic (> pH 7) sediments and soils from Table 12 to a great extent. The mean K_{oc} value including all measurements is 258 ± 257 L.kg^{-1} (c.v. = 99%), the mean of K_{oc} values for soils and sediments with pH >7 is 176 ± 59 L.kg^{-1} (c.v. = 34%).

Table 13. Statistical summary of K_{oc} values from Table 12. K_{oc} values and standard deviations given in L.kg^{-1}.

	All K_{oc} values	K_{oc} from soils and sediments with pH ≥ 7	K_{oc} from soils and sediments with pH < 7
mean	325	186	602
standard deviation	257	59	279
c.v.	99%	34%	50%
n	15	10	5
geometric mean	258	176	556

For the aquatic compartment, the geometric mean K_{oc} value of 176 L.kg^{-1} (pH ≥ 7 sediments) would be suitable, since the pH of the majority of Dutch surface waters is higher than 7. Using F_{oc} = 0.1 (for EU-standard suspended matter), this gives a $K_{p,\ susp\text{-}water}$ of 17.6 or a log $K_{p,\ susp\text{-}water}$ of 1.25. Since derivation of EQS for sediments is triggered by a log $K_{p,\ susp\text{-}water}$ value > 3, derivation of a sediment EQS for DNOC is not triggered.
In order to derive EQSs for soil using equilibrium partitioning (EqP), we propose to use the geometric mean K_{oc} value for soils and sediments of 556 L.kg^{-1} (log K_{oc} = 2.75) derived using the data for more acidic soils and sediments.

In aerobic soil degradation (laboratory) studies, DT50 (dissipation) values of 4 and 15.5 days were found (20-22°C). After 80 days at 20°C, 60-65% mineralisation was observed ($^{14}CO_2$). Bound residue amounted to 35% at 5 days of incubation, decreasing to 24% at 24 days, while another study showed 22 and 37% bound residue after 7 days (Luttik and Linders, 1990). Potential for degradation in aquifers was shown under aerobic conditions (Broholm *et al.*, 2001) and anaerobic conditions (Arildskov *et al.*, 2001), although the latter study suggest abiotic degradation as the removal process. Resistance against biodegradation under methanogenic conditions in the presence of a heterogeneous anaerobic microbial population from a municipal digester was reported by O'Connor and Young (1989). Long term inhibition (incubation during 69 days) of methane formation by DNOC was also shown under these conditions.

2.5.4 Use

A variety of uses is mentioned in Tomlin (2002): ‘Control of overwintering stages of aphids, suckers, ermine moths, winter moths, tortrix moths, cherry blossom moths, scale insects, and spider mites on pome fruit trees, stone fruit trees, and soft fruit bushes. Control of annual broad-leaved weeds in cereals, maize, legumes, flax, tree fruit, bush fruit, hops, and grass-seed crops. Also used as a desiccant for leguminous seed crops; for destruction of potato haulms; and for chemical stripping of hops.’

Products containing DNOC as an active ingredient are no longer on the market in the Netherlands. This is a consequence of the EC decision on withdrawal of authorisations for plant protection products containing DNOC (EC, 1999). In September 1999, the admission of the last registered products was withdrawn in the Netherlands, allowing for use of remaining stocks until June 2000.

2.6 Aniline

2.6.1 Identity

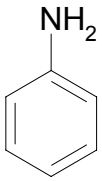

Figure 7. Structural formula of aniline.

Table 14. Identification of aniline.

Parameter	Name or nr.	Source
Chemical name	aminobenzene, benzeneamine, benzenamine	Mackay *et al.*, 2000
Common/trivial/other name	aniline	
CAS nr.	62-53-3	ECB, 2005
EC nr.	200-539-3	ECB, 2005
SMILES code	Nc(cccc1)c1	
INS priority nr.	162	

2.6.2 Physico-chemical properties

Table 15. Physico-chemical properties of aniline. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	93.13		MDL INformation Systems, 1997
Water solubility	[mg.L^{-1}]	**35000**	no information on method	EC, 2004a
		36000	25°C;experimental	Anonymus, 2005c
pK_a	[-]	4.63[a]	25°C	Lide, 1997
		4.60[a]	25°C	BioByte, 2006; Physprop
log K_{ow}	[-]	**0.9**	20°C; shake flask	EC, 2004a
		0.91	ClogP	BioByte, 2006
log K_{oc}	[-]	**2.61**[b]		EC, 2004a
Vapour pressure	[Pa]	**40**	20°C; method unknown	EC, 2004a
		106	25°C; mean of Antoine and Grain methods	US EPA, 2004
		65	25°C; experimental	Anonymus, 2005c
Melting point	[°C]	**-6.2**	method unknown	EC, 2004a
		-5.98-6.3	range of reported values	Mackay *et al.*, 2000
Boiling point	[°C]	**184.4**		EC, 2004a
		184-186	range of reported values	Mackay *et al.*, 2000
Henry's law constant	[Pa.m^3.mol^{-1}]	**0.106**		EC, 2004a
		0.192	calculated; bond method	US EPA, 2004
		0.22	calculated; group method	US EPA, 2004
		0.67	calculated from estimated P and S	US EPA, 2004
		0.21	experimental	Anonymus, 2005c
		12.16	measured; quoted value	Mackay *et al.*, 2000
		13778	quoted value	Mackay *et al.*, 2000

[a] pK_a for the protonated aniline species: C_6H_5-NH_3^+ + H_2O ↔ C_6H_5-NH_2 + H_3O^+.
[b] K_{oc} = 410 L.kg^{-1}. This K_{oc} is one of the K_{oc}'s derived from a distribution experiment and was determined in a sterile soil. In another sterile soil, a K_{oc} of 130 L.kg^{-1} was determined. Equilibrium in the sterile soils was reached after 120 hours. K_{oc} values determined in non-sterile soils were 310 and 910 L.kg^{-1}, equilibrium was attained after 60 hours. Aniline is degraded partly before adsorption and the distribution constants for the degradation products (azobenzene, azoxybenzene, phenazine) are much higher. Therefore, the constants determined in nonsterile soils seem to be overestimated (EC, 2004a, p. 25).

2.6.3 Behaviour

Information in this section is taken from the EU-RAR (EC, 2004a).
Aniline is readily biodegradable in standard tests under aerobic conditions, but not easily biodegradable under anaerobic conditions. In surface water studies, degradation and also mineralisation of aniline is observed. In lake water incubated at 29°C, a mineralisation half-life value of 5 days was observed for the concentration range 5 ng.L^{-1} to 5 µg.L^{-1}. The lowest half-life values for mineralisation in estuarine water were 33 days in summer (sunlight present), but 139 in summer (conducted in the dark). Half-life values in wintertime were 189 and 770 d, respectively. Half-life values for primary aniline degradation are much lower: 27 hours in summer with sunlight and 173 hours in summer in the dark. In seawater 15°C, half-life values of 11-31 days were measured at different concentrations.
Photolysis of aniline contributes to the removal rate in natural waters. A degradation rate constant could not be derived from the available information, but data show half-life values of 4 to 11 hours under spring or summer conditions in the upper layer of surface waters. Hydrolysis of aniline is expected to be of minor relevance based on molecular structure.
The few studies cited in the EU-RAR indicate relatively rapid biodegradation of aniline in soils. Biodegradation rates in soil are influenced by irreversible sorption of aniline. The amine group is thought to form covalent bonds with soil humic acid constituents like aldehyde- and keto-groups, but also double bonds. Since sorption of aniline appears partly irreversible, EqP theory does not apply, strictly spoken. However, EqP is the only methodology available to calculate sediment or soil concentrations in case toxicity data for species representative for those compartments are lacking. The K_{oc} of 410 L.kg^{-1} was selected in the EU-RAR to perform EqP calculations and will also be used in this report.

2.6.4 Use

Information in this section is taken from the EU-RAR (EC, 2004a).
Aniline is manufactured by reduction of nitrobenzene using iron and acetic acid. As a further product, high-grade synthetic iron oxides are produced which as used as pigments. A more modern method to produce aniline is catalytic reduction of nitrobenzene. For Western Europe, a total production capacity for aniline of 649,000 tonnes per year in 1989 is reported, while the production volume was 500,000 tonnes in 1990. An amount of 65,000 tonnes were imported and 5,000 tonnes were exported in the same year (1990).
Aniline is exclusively used as an intermediate in the chemical industry. It can be a residual component of dyes and adhesives. Aniline is processed by the chemical industry to 4,4'-methylenedianiline (MDA). MDA is synthesised by reaction of formaldehyde with aniline in the presence of hydrochloric acid. Aniline is processed to a series of compounds being used in the rubber industry, e.g. mercapto benzothiazole, diphenylguanidine, diphenylamine, aniline ketone condensates etc. Aniline is also used to process dyes, plant protection products and pharmaceuticals.
The following non-intentional releases have been identified in the EU-RAR: plant protection agents where aniline is formed as a degradation product; microbial reduction of nitrobenzene; rubber chemicals (degradation product); thermal degradation of polyurethanes; coal and oil industry; landfills.

2.7 Epichlorohydrin

2.7.1 Identity

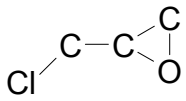

Figure 8. Structural formula of epichlorohydrin (source: ECB, 2005).

Table 16. Identification of epichlorohydrin.

Parameter	Name or nr.	Source
Chemical name	1-chloro-2,3-epoxypropane	ECB, 2005
Common/trivial/other name	epichlorohydrin; chloromethyloxirane; γ-chloropropylene oxide; 2-(chloromethyl) oxirane; (D,L)-α -epichlorohydrin	ECB, 2005 GDCh and German Chemical Society-BUA, 1992
CAS nr.	106-89-8	
EC nr.	203-439-8	ECB, 2005
SMILES code	O(C1CCl)C1	
INS priority nr.	56	

Table 17. Physico-chemical properties of epichlorohydrin. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	92.53		MDL INformation Systems, 1997
Water solubility	[mg.L^{-1}]	65000	20°C; pH neutral	ECB, 2000a
		66000	20°C	ECB, 2000a
		66000	25°C	ECB, 2000a
		65900	25°C; measured	Anonymus, 2005c
		35800	25°C; calculated from estimated; log K_{ow} 0.63	US EPA, 2004
pK_a	[-]	n.a.		
log K_{ow}	[-]	-0.21	calculated	Hansch & Leo (1989) cited in: GDCh and German Chemical Society-BUA, 1992
		0.3	20°C	ECB, 2000a
		0.45	measured at room temperature; MlogP value	BioByte, 2006; ECB, 2000a; Anonymus, 2005c; Deneer *et al.*, 1988
		0.46	MlogP value	BioByte, 2006
		0.58	calculated after Rekker (1977)	Deneer *et al.*, 1988]
		ca. 1	estimated after Freed *et al*. (1977)	Santodonato (1980) cited in: GDCh and German Chemical Society-BUA, 1992
		0.42	measured	Harder, 2002
		0.63	25°C; calculated, KOWWIN v1.67	US EPA, 2004
		0.39	25°C; calculated	Anonymus, 2006c
log K_{oc}	[-]	1.22	K_{oc}=17, QSAR estimate	ECB, 2000a, GDCh and German Chemical Society-BUA, 1992
		1	K_{oc}=10; calculated from regression between water solubility and K_{oc} (r^2=0.71)	GDCh and German Chemical Society-BUA, 1992
		0.652	K_{oc}=4.491 (calculated with PCKOCWIN v1.66)	US EPA, 2004
		2.09	K_{oc}=123, calculated from water solubility according to Lyman WJ et al (1982)	Anonymus, 2005b
		1.60	K_{oc}=40: calculated with log K_{ow}=0.45 and regression derived equation from Lyman WJ *et al*. (1990)	Anonymus, 2005b
		1.25	sorption QSAR for non-hydrophobics at room temperature	Sabljić and Güsten (1995) cited in: EC-JRC, 2003
Vapour pressure	[Pa]	1300	20°C	ECB, 2000a
		480	0°C; extrapolated value	Shell Industrial Chemicals (1986) cited in: GDCh and German Chemical Society-BUA, 1992
		1700	20°C	ECB, 2000a
		1600	20°C	Umwelt Bundes Amt, 1987
		2186	25°C; measured	Anonymus, 2005c
		1330	16.6°C	Ullmann (1986) cited in: GDCh and German Chemical Society-BUA, 1992
Melting point	[°C]	**-57.2**		Anonymus, 2005c
		-26		IPCS, 1984
Boiling point	[°C]	**116.11**		Anonymus, 2005c
Henry's law constant	[Pa.m^3.mol^{-1}]	2.43	20°C; calculated	ECB, 2000a
		3.08	calculated (P_v/S_w)	Anonymus, 2005c
		5.69	EPIWIN estimate bond method	US EPA, 2004
		13.48	EPIWIN estimate (P_v/S_w)	US EPA, 2004
DT50 hydrolysis	[d]	6.3	20°C; pH 4	ECB, 2000a; Kayen and von Hebel (1977) cited in: GDCh and German Chemical Society-BUA, 1992)
		7	15°C pH 4	ECB, 2000a
		6.2	20°C ; pH 7, aqueous solutions with 10% ethanol	Piringer (1980) cited in: Krijgsheld and Van der Gen, 1986
		6.5	20°C ; pH 5/6/7/8/9/10	ECB, 2000a; Kayen and von Hebel cited in GDCh and German Chemical Society-BUA, 1992
		8.0	20°C; pH 7, distilled water	ECB, 2000a

Parameter	Unit	Value	Remark	Reference
		8.2	20°C; pH 7; experimental	Mabey and Mill (1978) cited in GDCh and German Chemical Society-BUA, 1992
		5.3	20°C; pH 7, sea water (3% NaCl)	ECB, 2000a, Santodonato cited in Krijgsheld and Van der Gen, 1986
		6.5	20°C; pH 9	ECB, 2000a
		6.5	20°C; pH 10	ECB, 2000a
DT50 evaporation from water	[d]	2.1	20°C; estimated from S_w and P_v	Santodonato (1980) in Krijgsheld and Van der Gen, 1986
		0.5	25°C; with aeration; DT50 extrapolated, measured at t=4 h	Scientific Research Information International (1981) cited in: Krijgsheld and Van der Gen, 1986

n.a. = not applicable.

2.7.2 Behaviour

Epichlorohydrin is a highly volatile chemical. It is a colourless, mobile and very good soluble liquid with an irritating, chloroform-like odour. Since the molecule contains chiral carbon atom, the substance can occur in two enantiomeric forms. Both enantiomers will be present in equal amounts (racemic mixture). Epichlorohydrin is very reactive towards a wide variety of chemicals. Both the epoxide ring and the chlorine substituent are potentially electrophylic sites, the epoxide being the more reactive group.

In the aquatic environment, persistence of epichlorohydrin is classified as low, i.e. <1 week (Krijgsheld and Van der Gen, 1986). According to Krijgsheld and Van der Gen the elimination rate from environmental waters will mainly be determined by evaporation and hydrolysis. The Henry coefficient of 2.43 $Pa.m^{-3}.mol^{-1}$ can be converted to an air-water partitioning coefficient of 0.98 $dm^3.m^{-3}$, indicating that volatilization from water can contribute significantly. Based on estimates of Henry's law constant and K_{ow}, a fugacity model (Mackay Level I) predicts a theoretical distribution between atmosphere and hydrosphere of 54 and 46%, respectively (GDCh and German Chemical Society-BUA, 1992). The evaporation half-life has been calculated from its water solubility and vapour pressure for a 1 m water depth at 20°C and was estimated to be 2.1 days (Santodonato (1980) cited in Krijgsheld and Van der Gen, 1986). In an experimental study, epichlorohydrin evaporation was determined after a 4 hour period with an initial concentration of 100 ppm in a water cylinder at 25°C with aeration. The extrapolated half-life was found to be approximately 12 hours. Although the evaporation rate of epichlorohydrin will depend on environmental conditions, evaporation is expected to contribute significantly to the elimination of epichlorohydrin from the aquatic environment. The relative volatility of epichlorohydrin should be kept in mind in the evaluation of (laboratory) toxicity studies.
Hydrolysis of epichlorohydrin will lead to formation of 3-chloro-1,2-propanediol (alpha-chlorohydrin). At high pH values, further reaction will lead to glycerol. Epichlorohydrin may also react with various nucleophiles, e.g. chloride ions, to 1,3-dichloro-2-propanol. The half-life for hydrolysis of epichlorohydrin in distilled water (pH 7) and sea water (pH 7, 3% NaCl) at 20 °C has been calculated using kinetic relationships and was estimated to be 8.0 and 5.3 days (Santodonato (1980) cited in Krijgsheld and Van der Gen, 1986). In aqueous solutions (with 10% ethanol) and an initial concentration of 9.2 $mg.L^{-1}$ (pH 7, 20°C) a half-life of 6.2 days was determined experimentally. At pH 2.5 and 12 the half-life was 3.3 and 2.6 days, respectively (Piringer (1980), cited in Krijgsheld and Van der Gen, 1986).
Epichlorohydrin has been shown to be biodegradable in aqueous environments, although results are variable. A biodegradation study using activated sludge (initial concentration 169 $mg.L^{-1}$) from an industrial wastewater treatment plant, resulted in a 89% removal of the COD after 24 hours. However, 73% removal was found without activated sludge and was accounted for by loss through

evaporation (Matsui (1975), in GDCh and German Chemical Society-BUA, 1992). Another biodegradation study using microflora of a municipal wastewater treatment plant (Bridie *et al*. (1979), cited in Krijgsheld and Van der Gen, 1986) reported a 5 day biological oxygen demand (BOD_5) of 3% of the theoretical oxygen demand. After adaptation of the inoculate to epichlorohydrin this increased to 14%. The low BOD values indicate poor biodegradability for epichlorohydrin, although proper adaptation of the microflora may improve its rate of biodegradation. After14 days of incubation in OECD 301c test (freshwater, mixed culture) the degree of epichlorohydrin degradation is about 60% (MITI list (1986), cited in GDCh and German Chemical Society-BUA, 1992). In the modified MITI test, 60% degradation of epichlorohydrin in river water and 8% in sea water was found after 3 days (Kondo *et al*. (1988), cited in GDCh and German Chemical Society-BUA, 1992).
Direct photodegradation and oxidation are not expected to be important in the aquatic environment (Krijgsheld and Van der Gen, 1986). However, no information is available on the photochemical degradation of epichlorohydrin in water. In the atmosphere epichlorohydrin is expected to be degraded rapidly.

In conclusion, epichlorohydrin is a non-persistent chemical, which is not expected to bioaccumulate. Epichlorohydrin is probably carcinogenic to humans (Group 2A) (IARC, 1999a).

2.7.3 Use

Epichlorohydrin is used mainly for the manufacture of glycerol and unmodified epoxy resins and, to a lesser extent, in the manufacture of elastomers, water treatment resins, surfactants, ion exchange resins, plasticizers, dyestuffs, pharmaceutical products, oil emulsifiers, lubricants and adhesives (IPCS, 1984). The production capacity for epichlorohydrin in Europe has been estimated to be 205 kilo tonne/a (Scientific Research Information International (1981), cited in Krijgsheld and Van der Gen, 1986). GDCh, German Chemical Society-BUA (1992) gives an estimation of 240 kilo tonne/a.

2.8 1,2-Dibromoethane

2.8.1 Identity

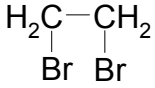

Figure 9. Structural formula of 1,2-dibromoethane.

Table 18. Identification of 1,2-dibromoethane.

Parameter	Name or nr.	Source
Chemical name	1,2-dibromoethane	ECB, 2005
Common/trivial/other name	ethylene dibromide; ethane, 1,2-dibromo-, 1,2-ethylene dibromide	
CAS nr.	106-93-4	
EC nr.	203-444-5	ECB, 2005
SMILES code	BrCCBr	
INS priority nr.	57	

2.8.2 Physico-chemical properties

Table 19. Physico-chemical properties of 1,2-dibromoethane. Bold values indicate values used in calculations. If more are data available, the geometric mean of reliable values is used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	187.87		Mackay *et al.*, 2000
Water solubility	[mg.L^{-1}]	**4099**	geometric mean, *n*=16, 2910-5130	Mackay *et al.*, 2000
		3910	at 25 °C, measured	Anonymus, 2005c
		4310		INERIS, 2005
		4300	at 30°C	IPCS, 1996
		2048	EPI estimate (fragment)	US EPA, 2004
pK_a	[-]	n.a.		
log K_{ow}	[-]	**1.96**		BioByte, 2006; Anonymus, 2005c
		2.01	EPI estimate	US EPA, 2004
log K_{oc}	[-]	1.699	calculated	Mackay *et al.*, 2000
		1.643	selected value	Mackay *et al.*, 2000
		1.80		Sablijć *et al.,* 2005
		1.82		INERIS, 2005
		1.64	EPI estimate	US EPA, 2004
Vapour pressure[a]	[Pa]	**1493**	at 25°C	Anonymus, 2005c
		1470	at 25°C	IPCS, 1996
		1560	EPI estimate (mean of Antoine and Grain methods)	US EPA, 2004
		1466		INERIS, 2005
		1040-1560	range of quoted values	Mackay *et al.*, 2000
Melting point	[°C]	**9.9**		IPCS, 1996
		9.79-9.97	two reported values	Mackay *et al.*, 2000
Boiling point	[°C]	131.4		IPCS, 1996
		131.4	geometric mean, *n*=4, 131.0-131.6	Mackay *et al.*, 2000
Henry's law constant	[Pa.m^3.mol^{-1}]	**63.7**	geometric mean, *n*=7, 15.64-110.7	Mackay *et al.*, 2000
		66		INERIS, 2005
		42.9	20°C; estimate (P_v/S_w) from this table	This report
		132	EPIWIN estimate bond method	US EPA, 2004
		15.6	EPIWIN estimate group method	US EPA, 2004
		303	EPIWIN estimate (P_v/S_w)	US EPA, 2004

n.a. = not applicable.
[a]geometric mean 1476 used in calculations.

2.8.3 Behaviour

Information on behaviour of 1,2-dibromoethane is cited from EHC 177 (IPCS, 1996).
1,2-Dibromoethane is moderately hydrophilic. It has a low vapour pressure and moves slowly in the vapour phase. Soil temperature is important and may affect 1,2-dibromoethane movement in several ways. A rise in temperature increases the vapour pressure and decreases the solubility. This alters the phase distribution and results in an increase in the rate of diffusion of 1,2-dibromoethane through soils.
1,2-Dibromoethane persists in top soil at µg.kg^{-1} levels for at least 20 years, despite its predicted lability in the environment (high water solubility and low soil-water partition coefficient). 1,2-Dibromoethane can serve as a C_1 unit and energy source for some soil aerobic or anaerobic micro organisms. However, residual 1,2-dibromoethane is strongly bound to soil and can only be extracted by warming with polar solvents. Diffusion of residual 1,2-dibromoethane from soil to water is very slow and highly temperature-dependent.

2.8.4 Use

Information on the use of 1,2-dibromoethane is cited from two sources; the e-Pesticide manual (Tomlin, 2002) and EHC 177 (IPCS, 1996).

Tomlin:
'1,2-Dibromoethane is used to control nematodes, wireworms and other soil pests and in fumigation of mills, warehouses and households.' 'It is phytotoxic to green plants and germinating seeds.'
EHC 177:
'Major uses of 1,2-dibromoethane are as a lead scavenger in tetra alkyllead petrol and antiknock preparations, as a soil and grain fumigant, as an intermediate in the synthesis of dyes and pharmaceuticals, and as a solvent for resins, gums and waxes. Legislation banning the use of lead in gasoline and controlling the agricultural use of 1,2-dibromoethane has reduced world demand for 1,2-dibromoethane by at least 75%.'

2.9 Ethinylestradiol

2.9.1 Identity

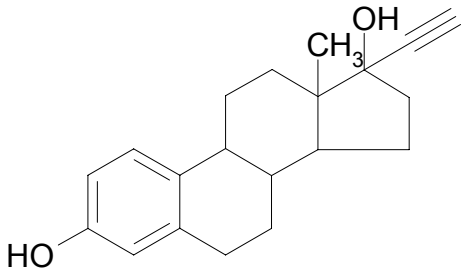

Figure 10. Structural formula of ethinylestradiol.

Table 20. Identification of ethinylestradiol.

Parameter	Name or nr.	Source
Chemical name	19-nor-17α-pregna-1,3,5(10)-trien-20-yne-3,17-diol	ECB, 2005
Common/trivial/other name	ethinylestradiol	ECB, 2005
CAS nr.	57-63-6	
EC nr.	200-342-2	ECB, 2005
SMILES code	OC(C#C)(C(C(C(C(c(c(cc(O)c1)C2)c1)C3)C2)C4)(C3)C)C4	
INS priority nr.	152	

2.9.2 Physico-chemical properties

Table 21. Physico-chemical properties of ethinylestradiol. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	296.41		MDL INformation Systems, 1997
Water solubility	[mg.L^{-1}]	**11.3**	measured, at 27°C	Anonymus, 2005c
		9.7	shake flask, at 25°C	Hurwitz and Liu, 1977
		3.1±0.03	shake flask, at 22°C	Yu *et al.*, 2004
		13.23	calculated; for 25°C; from log K_{ow} =4.68	US EPA, 2004
		48.42	calculated fragment method	US EPA, 2004
		19	cited from Schweinfurth *et al*., 1996	Young *et al.*, 2002
		4.8	cited from Tabak *et al*., 1996	Young *et al.*, 2002
		4.7	cited from Norpoth *et al*., 1996	Young *et al.*, 2002
pK_a	[-]	10.40±0.01	experimentally determined	Hurwitz and Liu, 1977
log K_{ow}	[-]	**3.67**	measured value; unpublished results, quality high	BioByte, 2006
		3.9±0.2	shake flask	Holthaus *et al.*, 2002
		4.15	method unknown, cited by many authors	Yu *et al.*, 2004; Ying *et al.*, 2003; Andersen *et al.*, 2005;

Parameter	Unit	Value	Remark	Reference
				Lai *et al.*, 2000
		3.86	calculated, ClogP	BioByte, 2006
		4.12	calculated; KOWWIN v1.67	US EPA, 2004
log K_{oc}	[-]	3.52[a]	average, measured in bed sediments (*n*=8)	Holthaus *et al.*, 2002
		2.99[a]	average, sediment and 2 soils (*n*=3)	Lee *et al.*, 2003
		3.31[a]	median, sewage sludge, several values, 95%CI = 3.16-3.46)	Clara *et al.*, 2004
		2.92[a]	average, sewage sludge (*n*=2)	Ternes *et al.*, 2004
		3.71[a]	average, soil and sediments (*n*=4)	Yu *et al.*, 2004
		3.32[a]	sewage sludge (*n*=1)	Andersen *et al.*, 2005
		3.72[a]	average, soil (*n*=4)	Ying and Kookana, 2005
		3.16[a]	average, soil (*n*=3)	Sarmah and Northcott, 2006
		3.38[a]	average, soil (*n*=4)	Hildebrand *et al.*, 2006
		4.68	calculated, PCKOCWIN v1.66	US EPA, 2004
Vapour pressure	[Pa]	3.56×10^{-7}	calculated, at 25°C; MPBPWIN v1.41	US EPA, 2004; Anonymus, 2005c
Melting point	[°C]	**171.12**	calculated; MPBPWIN v1.41	US EPA, 2004
		183		Anonymus, 2005c
Boiling point	[°C]	**411.21**	calculated; MPBPWIN v1.41	US EPA, 2004
Henry's law constant	[$Pa.m^3.mol^{-1}$]	**8.04×10^{-7}**	calculated; Henrywin v3.10	US EPA, 2004; Anonymus, 2005c
		2.18×10^{-6}	calculated; P_v/S_w	US EPA, 2004
		1.62×10^{-7}	calculated; P_v/S_w	EC, 2004b

n.a. = not applicable.
[a]see section 2.9.3.1 for more detail and calculation of final value.

2.9.3 Behaviour

After ingestion of the pill (contraceptive containing ethinylestradiol as active), the substance is subsequently excreted by humans in urine or faeces, either as ethinylestradiol or conjugated with glucoronide and/or sulphate. The latter is considered to be biologically inactive (Young *et al.*, 2002), but can be deconjugated by micro-organisms, e.g. in a sewage treatment plant. The unconjugated form is more abundant in effluents and rivers than the conjugated form (Layton *et al.*, 2000).

Andersen *et al*. (2004) reported concentrations of <1 – 4.8 $ng.L^{-1}$ in STP (sewage treatment plant)-influents and <1 – 5.2 $ng.L^{-1}$ in STP-effluents. They also reviewed a selection of recent literature, indicating that primary treatment alone resulted in limited or no removal from sewage. A long sludge retention time and secondary treatment significantly reduced the levels of ethinylestradiol, predominantly in the nitrification step. Jürgens *et al*. (2002) reported a DT_{50} in river water of 17 days, when administering 0.1 $mg.L^{-1}$ ethinylestradiol. The photolysis half-life in this experiment was calculated to be at least 10 days, assuming 12 hours of sunlight per day. Half-lives in activated sludge ranging from 1.3 to 12 hours were observed under aerobic conditions, while under anaerobic conditions half-lives were considerably longer (1.0 and 8.3 days, depending on the amount of mixed liquid suspended solids added).

2.9.3.1 Adsorption

Error! Not a valid bookmark self-reference. shows a summary of results obtained in various adsorption studies. Differences between adsorption constants do not appear to be related to the sorbent matrix. Therefore, log K_{oc} values were averaged per study and are presented as such in the table. The overall average of the log K_{oc} values in **Error! Not a valid bookmark self-reference.** is 3.34. This value for log K_{oc} will be used in further calculations.

Table 22. Summary of sorption constants for ethinylestradiol determined using various adsorbents.

Matrix	Calculation/study type	Average log K_{oc}	n[d]	Reference
river bed sediments	K_d, isotherm[a]	3.52[e]	8	Holthaus *et al.*, 2002
soil and sediments	K_d, isotherm[a]	2.99	3	Lee *et al.*, 2003
sewage sludge	K_d, isotherm[a]	3.31	1	Clara *et al.*, 2004
sewage sludge	K_d, point[b]	2.92	2	Ternes *et al.*, 2004
soil and sediments	K_f, isotherm[c]	3.71[f]	4	Yu *et al.*, 2004
sewage sludge	K_d, isotherm[a]	3.32	1	Andersen *et al.*, 2005
soil	K_d, point[b]	3.72	4	Ying and Kookana, 2005
soil	K_f, isotherm[c]	3.16	3	Sarmah and Northcott, 2006
soil	K_f, isotherm[c]	3.38	4	Hildebrand *et al.*, 2006

[a] K_d, isotherm: a linear or near linear isotherm relationship was observed, resulting in a K_d, from which K_{oc} was determined.
[b] K_d, point: K_d determined at a single concentration.
[c] K_f, isotherm: a Freundlich isotherm showing a linear or near linear relationship (the Freundlich constant, $^1/_n$, being close to unity) was observed, from which the generalisation could be made that K_f represents K_d. K_f was thus recalculated to K_{oc}
[d] n = number of K_{oc} values averaged per study.
[e] Results obtained with suspended sediments excluded.
[f] Two results with $^1/_n$ of 0.67 and 0.61 were excluded from average.

Holthaus *et al*. (2002) experimentally determined log K_{oc} values in suspended sediments and bed sediments. The values determined in suspended sediments (average 3.04) were not included in our average because a very short equilibration time (1 hour) was used and, moreover, the authors reported several practical difficulties. From the study of Yu *et al*. (2004), those K_f values that showed strong deviation from isotherm linearity ($^1/_n$ of 0.667 and 0.612) were excluded. A K_{oc} from Ying *et al*. (2003) was excluded for the same reason ($^1/_n$ = 0.46). Yamamoto *et al*. (2003) reported ethinylestradiol sorption constants on humic and fulvic acids, determined at a single concentration. K_{oc} values were consistently higher (roughly 1 order of magnitude) than those obtained in the various studies. Because the representativeness of the pure humic or fulvic acids to the field situation for soils and sediments (complete matrices) is disputable, the values from this study were excluded from the average. Although ethinylestradiol could not unambiguously be assigned to one of the QSAR (quantitative structure activity relationship)-classes of Sabljić *et al*. (1995), using the QSAR for nonhydrophobics or phenols, log K_{oc} values of 2.80 or 3.21 are calculated, respectively, of which the phenol-class estimate (3.21) is in the same order of magnitude as the experimental values.

2.9.4 Use

Ethinylestradiol is a synthetic steroid that is used in human medicine to treat various gynaecological disorders, post-menopausal breast cancer and acne, but its main use is in oral contraceptives, usually in combination with a synthetic progestin. Its concentration in the contraceptive pill may vary from 20 to 50 µg, with 35 µg being the most commonly prescribed dose (Archand-Hoy *et al*., 1998 as cited in Young *et al*., 2002). In the Netherlands, an estimated number of 1.4 million women use contraceptive pills on the basis of which a daily emission of 50 g has been calculated (Health Council of the Netherlands, 1992 as cited in Vethaak *et al*., 2002).

2.10 Methyl bromide

2.10.1 Identity

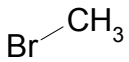

Figure 11. Structural formula of methyl bromide.

Table 23. Identification of methyl bromide.

Parameter	Name or nr.	Source
Chemical name	bromomethane, monobromomethane	ECB, 2005
Common/trivial/other name	methyl bromide	ECB, 2005
CAS nr.	74-83-9	
EC nr.	200-813-2	ECB, 2005
SMILES code	BrC	
INS priority nr.	172	

2.10.2 Physico-chemical properties

Table 24. Physico-chemical properties of methyl bromide. Bold values indicate values used in calculations. If no value is bold the geometric mean of the different values is taken.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	94.94		MDL INformation Systems, 1997
Water solubility	[mg.L^{-1}]	13.4[a]	at 25°C; purity >99.9%	Visser and Linders, 1992
		13.4[a]	at 25°C; purity unknown	Visser and Linders, 1992
		16 – 18.04[a]	at 20°C; purity unknown	Visser and Linders, 1992
		18500	at 20°C; purity unknown	Hertel and Kielhorn, 1995
		15400	at 25°C; purity unknown	Hertel and Kielhorn, 1995
		18000	at 20°C; purity unknown	Hertel and Kielhorn, 1995
		16000	at 20°C; purity unknown	Hertel and Kielhorn, 1995
		15200	measured, at 25°C	Anonymus, 2005c
		16100	at 25°C	OECD, 2002
		900	20°C	ATSDR, 1992
		13400-18100	20°C	ATSDR, 1992
		13000	20°C	ATSDR, 1992
		11970	EPIWIN estimate from log K_{ow}	US EPA, 2004
		21705	EPIWIN estimate from fragments	US EPA, 2004
		15223		Mackay *et al.*, 2000
pK_a	[-]	n.a.		
log K_{ow}	[-]	0.076	purity unknown	Visser and Linders, 1992
		1.94	measured, 25°C	OECD, 2002
		1.18	estimate	US EPA, 2004
		1.19	MlogP	BioByte, 2006; Anonymus, 2005c, Hertel and Kielhorn, 1995;Mackay *et al.*, 2000
log K_{oc}	[-]	2.236[b]	soil, loamy sand, Naaldwijk	Mackay *et al.*, 2000
		2.241[b]	soil, loam, Aalsmeer	Mackay *et al.*, 2000
		2.215[b]	peaty clay, Boskoop	Mackay *et al.*, 2000
		0.62[c]	soil; sandy loam	Visser and Linders, 1992
		0.59[c]	soil; sandy loam	Visser and Linders, 1992
		0.62[c]	soil; loam	Visser and Linders, 1992
		1.155	EPIWIN estimate	US EPA, 2004
Vapour pressure	[Pa]	**2.16×10^5**	experimental	Anonymus, 2005c
		1.8×10^5-2.57×10^5	range of values, mostly estimates, unclear if experimental	Mackay *et al.*, 2000
		1.89×10^5	at 20°C; purity >99.9%	Visser and Linders, 1992
		2.3×10^5	at 25°C; purity unknown	Visser and Linders, 1992

Parameter	Unit	Value	Remark	Reference
		1.84×10[b]	at 20°C; purity unknown	Visser and Linders, 1992
		9.12×10[4]	at 20°C; purity unknown	Visser and Linders, 1992
		1.893x10[3]	at 20°C; purity unknown	Hertel and Kielhorn, 1995
Melting point	[°C]	-94.07 − -93.00-	range of reported values	Mackay *et al.*, 2000
		-93	purity unknown	Visser and Linders, 1992
Boiling point	[°C]	3.55-4.60		Mackay *et al.*, 2000
		3.5 – 4	purity >99.9%	Visser and Linders, 1992
		4.5	purity unknown	Visser and Linders, 1992
		3.56	purity unknown	Visser and Linders, 1992
Henry's law constant	[$Pa.m^3.mol^{-1}$]	744[c]	experimental	Anonymus, 2005c
		631[d]	experimental	Mackay *et al.*, 2000
		533 – 20262[e]	range of calculated values	Mackay *et al.*, 2000
		550	no details given	Visser and Linders, 1992
		533	calculated using atmospheric pressure	Hertel and Kielhorn, 1995
		632		OECD, 2002

n.a. = not applicable.
[a]Erroneous values. An error in units ($mg.L^{-1}$ instead of $g.L^{-1}$) seems to have been made, since all other values and estimates are roughly a factor of 1000 higher than the values from Visser and Linders. The latter values will therefore not be considered in this ERL derivation.
[b]A log K_{oc} of 2.2 does not correspond with a reliable log K_{ow} estimate of 1.19. These values are most likely incorrectly cited as log K_{oc}. This parameter should presumably be K_{oc}. Original reference is not listed in Mackay, data can therefore not be validated and will not be used for ERL derivation.
[c]Geometric mean value of **0.606** will be used for ERL derivation.
[d]Selected value is **685** $Pa.m^3.mol^{-1}$ as geometric mean of 744 and 631.
[e]Mackay *et al*. (2000) report a broad range of values (326.8, 533, 621, 652, 652, 1317, 10689, 19958, 20268) without explanation. However al these values are estimates. The selected value will be based on experimental values.

2.10.3 Behaviour

Methyl bromide is a gas at temperatures above 3 to 4 °C. It is therefore used in compressed form (gas cylinders) as a liquid. Due to its volatility, methyl bromide will readily evaporate from water: its Henry coefficient of 550 $Pa.m^{-3}.mol^{-1}$ (Table 24) can be converted to an air-water partitioning coefficient K_{aw} of 0.22. First order half-life values for hydrolysis in water vary from 30 days at pH 3 to 12 days at pH 7 as determined in buffer solutions (18°C). In natural well water half-lives of 36 to 51 days were found in the range pH 7.4-7.8 (18°C). Aqueous photolysis under irradiation with natural light occurred with a half-life of 35-47 days at 20°C (All aquatic fate data: Visser and Linders, 1992).
When methyl bromide is used for soil disinfection, 70-90% is expected to diffuse to the atmosphere (Visser and Linders, 1992). Methyl bromide is the major source of inorganic bromine in the stratosphere. Reactive bromine contributes to stratospheric ozone depletion. Methyl bromide is contributes significantly to stratospheric ozone depletion on a global basis (UNEP/WMO, 2002). However, the majority of methyl bromide released into the atmosphere is derived from natural sources like macro algae, phytoplankton, fungi, higher plants and wetlands (Goodwin *et al.*, 2001).

2.10.4 Use

Methyl bromide is applied as a fumigant insecticide and nematicide. It is a multi-purpose fumigant used for insecticidal, acaricidal, and rodenticidal control in mills, warehouses, grain elevators, ships, etc., and in stored products; soil fumigation for control of insects, nematodes, soil-borne diseases, and weed seeds; and glasshouse and mushroom-house fumigation. It is extremely phytotoxic. Currently, there is only one authorised biocidal product containing methyl bromide on the market in the Netherlands and no plant protection products. The registered product, 'METHYL BROMIDE 100 voor ruimte ontsmetting', is methyl bromide in gaseous form. It is used against insects, mites and nematodes in quarantine and pre-shipment treatments (QPS) and in strawberry mother plants. From September 1, 2006 onwards, only its use as a plant protection product is allowed and biocidal application will no longer be admitted. The European Commission has decided that pre-shipment treatments are to be regarded as a plant protection product-application. It is intended to alter the application as a biocide to that of plant protection product (CTB, 2005b). Use for pre-shipment

treatment takes place in the harbour of Rotterdam, where dunnage wood in containers is treated in order to prevent spreading of exotic insects.

2.11 6PPD

2.11.1 Identity

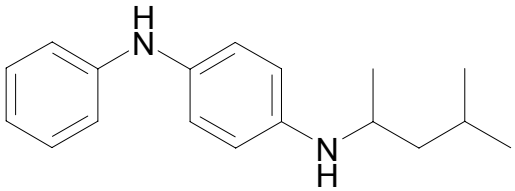

Figure 12. Structural formula of 6PPD (source: ECB, 2005).

Table 25. Identification of 6PPD.

Parameter	Name or nr.	Source
Chemical name	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	ECB, 2005
Common/trivial/other name	p-Phenylenediamine, N-(1,4-dimethylbutyl)-N'-phenyl; 4-[dimethylbutylamino]diphenylamine, 6PPD, Santoflex ® 6PPD; Santoflex ® 13, Vulkanox ® 4020, Accinox ® ZC, Antozite ® 67ZP, Flexzone ® 7P, Wingstay ® 300, UOP ® 588, Permanax 6PPD	US EPA, 2003
CAS nr.	793-24-8	
EC nr.	212-344-0	ECB, 2005
SMILES code	N(c(ccc(Nc(cccc1)c1)c2)c2)C(CC(C)C)C	
INS priority nr.	192	

2.11.2 Physico-chemical properties

Table 26. Physico-chemical properties of 6PPD. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	268.41		MDL INformation Systems, 1997; Anonymus, 2005c
Water solubility	[mg.L^{-1}]	1.88	calculated; for 25°C; from log K_{ow} =4.68	US EPA, 2004; Anonymus, 2005c
		2.83	calculated fragment method	US EPA, 2004
		1.1	no further information	ECB, 2000c; GDCh and German Chemical Society-BUA, 1998
		ca. 1	at °C; measured	OECD, 2004; GDCh and German Chemical Society-BUA, 1998
		1.1[a]	23°C, dark; valid without restriction (US EPA)	US EPA, 2003
		1.86[a]	25°C; valid without restriction (US EPA)	US EPA, 2003
pK_a	[-]			
log K_{ow}	[-]	4.68	calculated; KOWWIN v1.67	US EPA, 2004; OECD, 2004; Anonymus, 2005c
		4.77	25°C, dark; shake flask; 'valid with restrictions' (US EPA)	US EPA, 2003
		5.41	calculated, ClogP	BioByte, 2006; ECB, 2000c
log K_{oc}	[-]	**4.48**	calculated, QSAR for predominantly hydrophobics	EC-JRC, 2003
		4.84	calculated, PCKOCWIN v1.66	US EPA, 2004; OECD, 2004
Vapour pressure	[Pa]	8.53×10^{-4}	measured at 162°C	US EPA, 2003
		6.57×10^{-4}	calculated; MPBPWIN v1.41	US EPA, 2004, Anonymus, 2005c
		6.85×10^{-3}	calculated	OECD, 2004
Melting point	[°C]	45[b]	measured	US EPA, 2003

Parameter	Unit	Value	Remark	Reference
		46-50.1[b]	measured	US EPA, 2003
		45-48[b]	measured	ECB, 2000c; OECD, 2004
		50	no further information	ECB, 2000c
		121.50	calculated; MPBPWIN v1.41	US EPA, 2004
Boiling point	[°C]	230	at 13.3 hPa; measured	ECB, 2000c; OECD, 2004
		>350	at 1013 hPa; measured	US EPA, 2003
		369.67	calculated (at 1013 hPa); MPBPWIN v1.41	US EPA, 2004
Henry's law constant	[Pa.m^3.mol^{-1}]	3.40×10^{-4}	calculated; Henrywin v3.10	US EPA, 2004
		9.39×10^{-2}	calculated; P_v/S_w	US EPA, 2004
		3.43×10^{-4}	calculated	Anonymus, 2005c
		9.33×10^{-2}	calculated; using selected P_v/S_w from this table	this report
		1.84	calculated	GDCh and German Chemical Society-BUA, 1998

[a]Selected value is **1.23 mg.L^{-1}**, which is the geometric mean of these values after recalculation to 20°C using the Arrhenius equation (E_a of 2.7×10^4 J.mol^{-1}).
[b]Selected value is **47.6°C**, which is the arithmetic mean of the minimum (45) and maximum (50.1) value of all ranges found.

2.11.3 Behaviour

This content of this section is cited from OSPAR[1] Commission (2005), OECD SIDS[2] (2004), IUCLID[3] (ECB, 2000c) and BUA[4] 208 (GDCh and German Chemical Society-BUA, 1998).
Abiotic degradation of 6PPD in water is indicated by several studies. A half-life of approximately 1 day at 25°C in pure water is reported; 60% degradation was observed after 25 hours in deionised, diluted aqueous solution; a half-life of 3-4 hours was measured in pH 7 buffered, deionised, diluted aqueous solution. Half-life values of 6.8 hours in sterile deionised water and of 3.9 hours in sterile river water are also reported. Presence of oxygen and (traces of) heavy metals enhance degradation rates. A half-life of several hours was reported in algal medium. At pH 2 in the cold, 6PPD was stable for weeks, but at neutral or basic pH, degradation occurred within a few hours. In a river water die-away study, 97% degradation was observed after 22 hours.
In Anonymus (2006d), results of several hydrolysis tests with 6PPD are presented. At pH7 and 25°C, 93% degradation was observed after 24 hours of exposure, and 99% degradation was observed after 7 days. A more extensive hydrolysis study is summarised in Table 27.

Table 27. Hydrolysis of 6PPD under different conditions (Anonymus, 2006d).

pH	light/dark	% degradation	time	notes
5	dark	51.5	54.3	
7	dark	64.3	6.3	deionised water
7	dark	69.8	5.7	well water
9	dark	90.4	6.7	
5	light	73.3	26.7	
7	light	85.6	3.7	well water
9	light	90.0	6.7	

This experiment confirms the findings stated in the above section and indicate that sunlight enhances degradation rates of 6PPD at pH 7.

6PPD is photodegraded rapidly in air by OH radicals, its calculated half-life value in air is 1 hour. No data on photolysis in water are available, but 6PPD is expected to undergo rapid photolysis in water as well. UV absorption maxima are measured at 291 and 350 nm.

[1] OSPAR = Olso and Paris convention.
[2] OECD = organisation for economic co-operation and development, SIDS = screening information data set.
[3] IUCLID = international uniform chemical information database.
[4] BUA = advisory committee on existing chemicals of environmental relevance (German institution).

Ready biodegradability tests showed that 6PPD was degraded, showing results of 2% degradation (BOD), 13-40% mineralisation in 28 days and 7% mineralisation in 32 days. However, since the 10 day window was not fulfilled, 6PPD is classified as 'not ready biodegradable'. No data on degradation in soil have been found.

2.11.4 Use

This content of this section is cited from OECD SIDS (2004) and BUA 208 (GDCh and German Chemical Society-BUA, 1998).
6PPD was produced in the Federal Republic of Germany at a rate of 5000-10 000 tonnes.y^{-1} between 1990 and 1993. In 2004 it was manufactured at only one site in Germany (Bayer AG, Brunsbüttel). Other manufacturers in Europe (reported in 1994) were AKZO in Great Britain, Monsanto in Great Britain and Belgium, Uniroyal in Italy and Petrimex in Slovakia. Present manufacturers according to ESIS (European chemical substances information system) are Bayer AG in Germany and Monsanto Europe in Belgium. Bayer AG estimated the worldwide market volume in 2001 at 140 000 tonnes.y^{-1}.

6PPD is used as rubber antidegradant. It is a radical scavenger and acts as antioxidant and antiozonant, thus protecting rubber against wear and ageing. The main area of application is the rubber sector, with the majority of the manufacturing volume going into tyres. New tyres for passenger cars contain up to 1% of 6PPD (and IPPD: N-isopropyl-N'-phenyl-1,4-phenylene diamine, CAS No. 101-72-4), lorry tyres contain up to 2%. Rubber antioxidants are also used in articles like conveyor belts, spring parts, sealings, drive-belts, hoses, cables and gaskets. Values given for the fraction of 6PPD that is not bound to the rubber polymer matrix are ≥ 80% and 55-80%. This fraction is generally extractable with water or organic solvents.

Emission during production can occur, although incineration in combination with particle filters and waste water treatment will minimise loss to the environment. During use, release to the environment can occur through migration to the surface, leaching, volatilisation and chemical reaction with ozone, oxygen and other radicals. This might cause indirect introduction into the environment. Additionally, leaching and rotting of rubber articles at the waste stage contributes to emission.

2.12 3,3'-Dichlorobenzidine

2.12.1 Identity

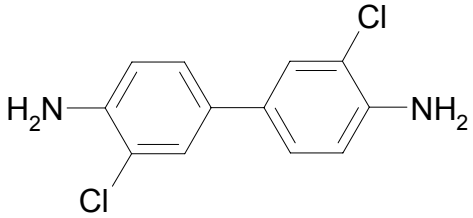

Figure 13. Structural formula of 3,3'-dichlorobenzidine.

Table 28. Identification of 3,3'-dichlorobenzidine.

Parameter	Name or nr.	Source
Chemical name	3,3'-dichlorobiphenyl-4,4'-ylenediamine	ECB, 2005
Common/trivial/other name	3,3'-dichlorobenzidine, *o,o*' –dichlorobenzidine, 3.3'-dichloro-biphenyl-4,4' diyldiamine (IUPAC), Curithane	ECB, 2005
CAS nr.	91-94-1	
EC nr.	202-109-0	ECB, 2005
SMILES code	Nc(c(cc(c(ccc(N)c1Cl)c1)c2)Cl)c2	
INS priority nr.	205	

2.12.2 Physico-chemical properties

Table 29. Physico-chemical properties of 3,3'-dichlorobenzidine. Bold values indicate values used in calculations.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g.mol^{-1}]	253.13		MDL INformation Systems, 1997
Water solubility	[mg.L^{-1}]	3.11[a]	measured, at 25±0.2°C	Banerjee *et al.*, 1980
		3.99[a,b]	measured; pH 6.9; 22°C as dihydrochloride	Sikka *et al.*, 1978; Banerjee *et al.*, 1978; Mackay *et al.*, 2000
		15.0	calculated fragment method	US EPA, 2004; Anonymus, 2005c
		41.1	calculated; for 25°C; from log K_{ow} =4.68	US EPA, 2004
		ca. 35	at 20°C	ECB, 2000b
		ca. 3	at 25°C	ECB, 2000b
		50	at 30°C and pH 7	ECB, 2000b
pK_a	[-]	1.6[c]	p$K_{a,1}$; method not reported	Cited by Nyman *et al.*, 1997
		3.2[b,c]	p$K_{a,2}$; experimental; method not reported	Nyman *et al.*, 1997
		2.18	calculated	Anonymus, 2006c
		2.3	calculated from pK_b of 11.7	Mackay *et al.*, 2000
log K_{ow}	[-]	3.02		Mackay *et al.*, 2000
		3.35	calculated	Mackay *et al.*, 2000
		3.21	calculated; KOWWIN v1.67	US EPA, 2004; Anonymus, 2005c
		3.5	method not reported	Cited by Nyman *et al.*, 1997
		3.51	measured; MlogP	Banerjee *et al.*, 1980; BioByte, 2006; Mackay *et al.*, 2000
		3.57	calculated, ClogP	BioByte, 2006
		3.64	calculated	Mackay *et al.*, 2000
		3.5	at 23°C and pH 8.7; shake flask	ECB, 2000b
		3.78	at 25°C; spectrophotometrical determination	ECB, 2000b
log K_{oc}	[-]	3.87	calculated, PCKOCWIN v1.66	US EPA, 2004; Meylan and Howard, 1992; Mackay *et al.*, 2000
		33.19	calculated; most likely erroneously reported	Mackay *et al.*, 2000
		3.30	calculated	Mackay *et al.*, 2000
		4.35	experimental, no further data	Meylan and Howard, 1992
		5.32	freshwater sediment; ^{14}C-DCB (water phase); $^{1}/_{n}$ = 0.96; r^2>0.98	Sikka *et al.*, 1978
		5.13	based on K_d value (determined at one concentration); ^{14}C-DCB (water phase)	Sikka *et al.*, 1978
		5.28	based on K_d value (determined at one concentration); ^{14}C-DCB (water phase)	Sikka *et al.*, 1978
		5.55	based on K_d value (determined at one concentration); ^{14}C-DCB (water phase)	Sikka *et al.*, 1978
		2.86	sediment; non labelled; experimental value; $^{1}/_{n}$ 0.63 (water phase analysed)	Nyman *et al.*, 1997
		2.92	sediment; non labelled; experimental value; $^{1}/_{n}$ 0.69 (water phase analysed)	Nyman *et al.*, 1997
		3.08	sediment; non labelled; experimental value; $^{1}/_{n}$ 0.66 (water phase analysed)	Nyman *et al.*, 1997
		1.86	sediment; non labelled; experimental value; $^{1}/_{n}$ 0.48 (water phase analysed)	Nyman *et al.*, 1997
		3.21	sediment; non labelled; experimental value; $^{1}/_{n}$ 0.57 (water phase analysed)	Nyman *et al.*, 1997
		4.52	clay loam soil; ^{14}C-DCB; batch adsorption study; LSC water phase	Boyd *et al.*, 1984
		4.20	sand soil; batch adsorption study; LSC water phase	Boyd *et al.*, 1984

Parameter	Unit	Value	Remark	Reference
Vapour pressure	[Pa]	**3.41×10^{-5}**	calculated (25°C); MPBPWIN v1.41	US EPA, 2004; Anonymus, 2005c
		1.33×10^{-3}	estimated	Mackay *et al.*, 2000
		6×10^{-7}	at 20°C; no further information	ECB, 2000b
		6.1×10^{-7}	at 20°C; no further information	ECB, 2000b
		6×10^{-3}	at 80°C; no further information	ECB, 2000b
Melting point	[°C]	155.54	calculated; MPBPWIN v1.41	US EPA, 2004
		132	no further information	Mackay *et al.*, 2000
		132.4	no further information	ECB, 2000b
		≥ 132.4	no further information	ECB, 2000b
		132-133	no further information	Anonymus, 2005c
Boiling point	[°C]	407.27	calculated; MPBPWIN v1.41	US EPA, 2004
		368	no further information	Anonymus, 2005c
		250	no further information	ECB, 2000b
		>250	no further information	ECB, 2000b
Henry's law constant	[$Pa.m^3.mol^{-1}$]	5×10^{-5}	calculated; P_v/S_w; 20-25°C	GDCh and German Chemical Society-BUA, 1989
		2.88×10^{-6}	calculated; Henrywin v3.10, bond method	US EPA, 2004; Mackay *et al.*, 2000
		5.18×10^{-6}	calculated; Henrywin v3.10, group method	US EPA, 2004
		2.10×10^{-4}	calculated; P_v/S_w	US EPA, 2004
		8.11×10^{-2}	calculated P_v/S_w	Mackay *et al.*, 2000 after Mabey *et al.*, 1982
		1.45×10^{-3}	calculated (20°C); EPI estimate P_v/ selected S_w (3.09 $mg.L^{-1}$) see text below table	this report

[a]The experimentally determined values of 3.11 $mg.L^{-1}$ (at 25°C) and 3.99 $mg.L^{-1}$ (at 22°C) were recalculated to 20°C using the Arrhenius equation (E_a of 2.7×10^4 $J.mol^{-1}$). This results in 2.59 and 3.70 $mg.L^{-1}$ of which the geometric mean (**3.09** $mg.L^{-1}$) will be used as selected value.
[b]Quoted as 4.00 by Mackay *et al*. (2000). However, Mackay cites Banerjee *et al*. (1978) who actually report 3.99.
[c]pK_a for the protonated aniline species: $R\text{-}NH_3^+ + H_2O \leftrightarrow R\text{-}NH_2 + H_3O^+$.

2.12.3 Behaviour

3,3-Dichlorobenzidine (DCB) is a very weak base, the two pK_a values for the NH_2 groups indicate that the molecule is uncharged at pH values around 7, i.e. in most natural waters.

Stability in water, soil and sewage sludge

IUCLID data (ECB, 2000b) indicate the following: DCB was hydrolytically stable in several experiments: (1) no degradation occurred during 30 days at 21°C in the dark in sterile aqueous solution; (2) no degradation occurred during 7 days at pH 2, 4.7, 7 and 10 at 4°C in aqueous solution. Photodegradation on silica gel showed 42% degradation in 17 h, resulting in CO_2 formation. The half-life for photolysis in water under artificial light (at 253 nm and 300 nm) was < 5 minutes and approximately 1.5 minutes under sunlight (Banerjee *et al.*, 1978). Reductive dechlorination of DCB in aqueous solutions was observed at wavelengths of 300-360 nm. Half-life values were in the order of minutes, and formation of 3-chlorobenzidine (MCB) and benzidine was confirmed (Nyman *et al.*, 2002). In two soil degradation studies, no dissipation was observed in 6.5 and 8 months, respectively. This is confirmed by results discussed in the Canadian Environmental Protection Act (CEPA, 1993), which indicated very slow degradation under both aerobic and anaerobic conditions. Boyd *et al*. (1984) observed only 2% mineralisation after 32 weeks of incubation in two aerobic soils (a clay loam and a sand); no mineralisation was observed after 1 year under anaerobic conditions. No major transformation products were identified in both soils. Half-life values of 10 to 80 days at 20°C were determined for the anaerobic degradation of DCB in lake sediments, depending on the sediment characteristics and initial DCB concentration (Nyman *et al.*, 1997). Half-life values of 16 to 22 days at 24°C and 34 to 62 days at 4°C were observed in a second study (anaerobic, freshwater, lake sediments). The observed degradation pathway was reductive dechlorination, as in the aqueous photolysis experiment, with formation of MCB and benzidine as metabolites as confirmed by mass spectrometric analysis

Although one study summarized in IUCLID showed that DCB was inherently biodegradable, this result was not corroborated in four other studies with activated sludge.

Sorption

DCB sorption to soil (exp. log K_{oc} of 4.35 vs. QSAR estimate 2.85) was underestimated by the general QSAR for nonhydrophobics (1995) and DCB was considered an outlier in that study. Cationic sorption may contribute to reversible sorption for ionisable species, although this is expected to be less relevant for DCB in view of its low pK_a values: at near neutral pH values, the majority of DCB molecules is uncharged. Irreversible sorption to soil is proposed to occur for aromatic amines (as well as other types of compounds; Weber *et al.*, 2001; Donaldson and Nyman, 2005; Lee *et al.*, 1997).
In a study by Donaldson and Nyman (2005), the mechanistic contribution of three sorption processes was investigated. Equations for sorption due to hydrophobic partitioning, cationic exchange and covalent binding of the amine group with organic matter were combined in a multi parameter model that adequately fitted the nonlinear DCB sorption in five sediments. All three (modelled) processes contributed to overall sorption in varying degree, depending on the sediment characteristics. The estimated contribution of partitioning to overall sorption ranged from 15% to 73%, that of covalent bonding ranged from 19% to 84%. Sorption isotherms for sediments with the same characteristics were also determined using the Freundlich model (Nyman *et al.*, 1997), which revealed a strong deviation from linearity ($^1/_n$ = 0.48 – 0.69). Normalisation of the obtained K_f values to organic carbon content of the sediments gives a log K_{oc} range of 2.9-3.2 with one outlier of 1.9. The Freundlich adsorption isotherm was better approximated by linearity in the studies of Boyd *et al*. (1984) and Sikka *et al*. (1978).

Since sorption of DCB seems to be partly irreversible, EqP theory does not apply, strictly spoken. Moreover, normalisation to organic carbon seems not appropriate since more parameters might contribute to overall sorption of DCB. However, EqP is the only methodology available to calculate sediment or soil concentrations in case toxicity data for species representative for those compartments are lacking. Averaging the available log K_{oc} values (n = 11, Nyman *et al.*, 1997; Sikka *et al.*, 1978; Boyd *et al.*, 1984) gives a mean value of 3.99 with a log standard deviation of 1.26. The mean log K_{oc} value of **3.99** will be used in ERL derivation.

2.12.4 Use

3,3-Dichlorobenzidine is used in the production of yellow and orange coloured (azo)pigments and azo dyes for use in printing ink, textile, paper, paint, rubber, plastic etc. The pigments and dyes contain a diazotised form of 3,3'-dichlorobenzidine. 3,3'-Dichlorobenzidine has some other uses, like that of intermediate in 3,3',4,4'-tetraaminobiphenyl production, as co monomer in the production of polyurethane elastomers, and as colour reagent of the detection of gold and of blood (1998;1989).

In 1983, 4200 tonnes of 3,3'-dichlorobenzidine were available in Western Europe, of which approximately 97-98% were used for pigment production and the rest for production of 3,3',4,4'-tetraaminobiphenyl (GDCh and German Chemical Society-BUA, 1989). For Germany, emission during production (out of purified waste water) was estimated to be less than 6 g per tonne; emission during processing was estimated at 200 grams per tonne. Residual 3,3'-dichlorobenzidine may account up to 90 mg.kg^{-1} of pigment. This residual 3,3'-dichlorobenzidine is not emitted into the environment since it is encased in insoluble pigment and remains immobilised (GDCh and German Chemical Society-BUA, 1989; Mensink *et al.*, 1998b).

In a survey on azo dyes (Mensink *et al.*, 1998a), it was reported that in the Netherlands, production of 'carcinogenic dyes' can be excluded. Based on surveys and interviews, it was concluded that the use of carcinogenic azo dyes by Dutch companies is also limited. The only use that was identified was colouring of mineral oil, like diesel oil and household oil, amounting to 140-200 tons (of dye)

per year on the Dutch market (1998). In the same study, the import of carcinogenic azo dyes was estimated to be 95 tons per year (excluding use in mineral oil), which is subsequently re-exported to other countries.

2.12.5 Carcinogenicity

3,3'-Dichlorobenzidine is a potential human carcinogen; it is categorised as a class 2B carcinogen in the International Agency for Research on Cancer (IARC) monograph (IARC, 1987a). DCB is defined as carcinogenic to animals. DCB is a structural analog of benzidine, which is carcinogenic to humans (IARC class 1); it is known to cause bladder cancer.
A major concern for human health comes from the use of azo dyes in applications like garments, footwear, paper, toys, ink, footwear, bed linen, tattoos, etc. Azo dyes can be transformed into amines, e.g. on the skin, in the intestine by bacteria and in the body. Many of the amines that can be derived from azo dyes, have carcinogenic properties, as does 3,3'-dichlorobenzidine. A cancer risk assessment for aromatic amines derived from azo dyes used in consumer products was performed by Zeilmaker *et al*. (Zeilmaker *et al.*, 1999; Zeilmaker *et al.*, 2000). In the Netherlands, the trade in products containing azo dyes that can form (a selected list of) aromatic amines is regulated in the Dutch Commodities Act Regulation as amended (Anonymus, 1998; Anonymus, 2003) .

3. Methods

The procedures followed for data collection and data selection differ for the various compounds investigated in this report. Two groups are distinguished. Group 1 comprises those compounds for which data and/or EQSs have been or are currently being generated in other frameworks. Those compounds for which only an *ad hoc*-MPC is available and for which no EQSs have been set form Group 2.

3.1 Group 1: compounds evaluated in other frameworks

This group contains the following six compounds: DNOC, p-*tert*-octylphenol, isodrin, benzo[*b*]fluoranthene, aniline, pentaBDE. The data availability of each of these compounds is outlined in the following sections.

3.1.1 Compounds for which national EQSs have already been set

DNOC. ERLs for DNOC were derived by Crommentuijn *et al*. (1997) and these values have been adopted as EQSs in the Netherlands. The EQS values for DNOC are reported in Table 30 in this section. Data collected for the ERL derivation by Crommentuijn *et al*. were also used for the ERL derivation in this report.

Table 30. Environmental quality standards set for DNOC.

$MPC_{water, dissolved}$ [$\mu g.L^{-1}$]	$MPC_{water, total}$ [$\mu g.L^{-1}$]	$NC_{water, total}$ [$\mu g.L^{-1}$]	$TV_{gw, dissolved}$ [$\mu g.L^{-1}$]	TV_{soil} [$\mu g.kg_{s.soil.}^{-1}$]	$MPC_{sediment}$ [$\mu g.kg_{s.sediment.}^{-1}$]	$TV_{sediment}$ [$\mu g.kg_{s.soil.}^{-1}$]
21	21	0.2	0.2	0.7	280	0.7

Source: RIVM (2006). MPC = maximum permissible concentration, NC = negligible concentration; TV = target value; s.soil = Dutch standard soil (10% o.m.); s.sediment = Dutch standard sediment (10% o.m.).

3.1.2 Compounds for which an EU-RAR is in draft status

A targeted environmental RAR for **p-*tert*-octylphenol** has recently been published by the Environment Agency (Brooke *et al.*, 2005) of the United Kingdom. It has been discussed at the third TC NES (technical committee for new and existing substances) in 2005, Ispra, Italy. Member states have been asked to comment on the UK report. p-*tert*-octylphenol is also prioritised in the WFD and EQS proposals are available (see section 3.1.4). Brooke *et al*. was used as data source for ERL derivation. No additional data search was performed.

Benzo[*b*]fluoranthene is one of the PAHs for which PNECs are derived in the draft EU-RAR on coal tar pitch. This EU-RAR has been discussed at the first TC NES of 2006, Ispra, Italy. Benzo[*b*]fluoranthene is also prioritised in the WFD and EQS proposals are available (see section 3.1.4). The EU-RAR was used as data source for ERL derivation. No additional data search was performed.

3.1.3 Compounds for which a finalised EU-RAR is available

For **pentaBDE** a finalised EU-RAR is available. Toxicity data from the EU-RAR are used for derivation of MPC_{soil}, $MPC_{groundwater}$ and SRC_{eco}s (ecotoxicological serious risk concentration). Since pentaBDE is prioritised in the WFD, a WFD-fact sheet and an EQS proposal are also available (see section 3.1.4). The WFD fact sheet and the EU-RAR were used as data source for ERL derivation. No additional data search was performed.

For **aniline**, a finalised EU-RAR is available. The data and PNECs in this document were used as the basis for ERL derivation. No additional data search was performed.

3.1.4 WFD prioritised compounds

PentaBDE, p-*tert*-octylphenol and **benzo[*b*]fluoranthene** are listed as priority compound within the WFD. A WFD fact sheet for each compound is available, in addition to a final EU-RAR for pentaBDE and a draft EU-RAR for p-*tert*-octylphenol and benzo[*b*]fluoranthene. We have used the underlying data from the EU-RARs for ERL derivation. No further data search for ecotoxicological data was employed.

For pentaBDE, an updated value for the human risk limit was retrieved during this project. We have used this value in the ERL derivation, leading to values different from the EQS proposals. For p-*tert*-octylphenol, the ERL derivation was based on the same data as used in the WFD fact sheet. Since the EQS for benzo[*b*]fluoranthene was proposed as an interim value in the WFD fact sheet and the EU-RAR for coal tar pitch (PCTHT) was nearly finalised, we have based the ERL derivation benzo[*b*]fluoranthene on the EU-RAR data.

3.1.5 Compounds with a legally binding standard

For **Isodrin**, no WFD-fact sheet is available. Isodrin is listed in Part B of Annex I (Environmental quality standards for priority substances and certain other pollutants) of the proposal of the daughter Directive COM (2006) 397 (EC, 2006a) of the WFD. A sum standard is presented for the four drins: aldrin, dieldrin, endrin and isodrin. This standard has been taken over from 88/347/EEC (EC, 1988), a daughter Directive of Directive 76/464/EEC (EC, 1976). The standards set for the group of drins are the AA-QS (annual average quality standard) of 0.010 $\mu g.L^{-1}$ for inland waters and of 0.005 $\mu g.L^{-1}$ for other surface waters (marine compartment). The daughter Directive proposal COM (2006) 397 (EC, 2006a) lists the MAC-EQS (maximum acceptable concentration-environmental quality standards) values for the drins as ‘not applicable’. The ERLs for water, listed in COM (2006) 397 will be binding once the Directive is adopted. Since isodrin has never been admitted to the Dutch market, it seems unnecessary to derive ERLs for soil and groundwater.

3.2 Group 2: compounds for which only an *ad hoc* MPC is available

Only an *ad hoc* MPC is available for epichlorohydrin, bromomethane, 1,2-dibromoethane, ethinylestradiol, 6PPD and 3,3’-dichlorobenzidine. An ERL derivation will be performed for these compounds according to INS guidance.
An online literature search was performed on TOXLINE: 1985 – 2001 (January) and Current contents from 1997 - 2005. For the methodology of data search, data selection and ERL derivation, we refer to INS guidance (Van Vlaardingen and Verbruggen, 2007).

4. Bioconcentration, trigger values, human toxicological threshold limits

Sections 4.1 to 4.6 report on the selected bioconcentration factor (BCF) values and biomagnification (BMF) values, where appropriate (trigger values for ERL_{water} derivation (as demanded in WFD framework), and the derivation of a human toxicological threshold limit (where appropriate), for Group 1 compounds (Group 1 as discerned in this report, see page 16). Sections 4.7 to 4.12 report on the same topics for Group 2 compounds (Group 2 as discerned in this report, see page 16).

4.1 PentaBDE

4.1.1 Bioconcentration

In the EU-RAR (EC, 2001), a BCF of 14350 $L.kg^{-1}$ is used, whereas in the WFD datasheet (Anonymus, 2004) a BCF of 27400 $L.kg^{-1}$ is used. Both BCFs are derived from the same study with carp. The higher BCF is chosen for QS-determination, as a matter of precaution.

4.1.2 Trigger values

Table 31. PentaBDE: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	4.75	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	27400[a]	[$L.kg^{-1}$]		experimental
BMF	16 – 20[b]	[-]		experimental
Log K_{ow}	6.57[c]	[-]		
R-phrases	Xn; R48/21/22, R64, N; R50/53	[-]		
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]A BCF of 27400 Lkg^{-1} is recalculated in the EU-RAR on basis of available study data. However, for EUSES (European union system for the evaluation of substances) -calculation the original BCF of 14350 $L.kg^{-1}$ is used and a remark is made that the higher, recalculated BCF is taken into account in the risk assessment. In the draft WFD-datasheet, QS for secondary poisoning is determined with the BCF of 27400 $L.kg^{-1}$. It is reported that this BCF is used according to the 'precautionary principle'.
[b]For *Gasterosteus aculeatus* (EC, 2004a).
[c]Used in EC (2004a) and WFD datasheet (Anonymus, 2004).

Remark on log $K_{p,\ susp\text{-}water}$
Both the EU-RAR and WFD-datasheet have derived the log $K_{p,\ susp\text{-}water}$ from the log K_{oc} of 5.75. This log K_{oc} was in turn determined using the log K_{ow} of 6.97 (see Table 3). This value is the highest of a range of values determined using the HPLC method. However, the log K_{ow} selected for risk assessment and QS derivation in both the RAR and WFD-datasheet, is the value of 6.57, determined using a generator column method. Hence, in both documents, the log $K_{p,\ susp\text{-}water}$ and equilibrium partitioning calculations do not correspond with the selected value log K_{ow}.

- PentaBDE has a log $K_{p,\ susp\text{-}water} > 3$; derivation of $MPC_{eco,\ sediment}$ is triggered.
- PentaBDE has a log $K_{p,\ susp\text{-}water} > 3$; expression of the MPC_{water} as MPC_{water} in suspended particulate matter is required.
- PentaBDE has a BCF > 100; assessment of secondary poisoning is triggered.

- PentaBDE has an R64 (may cause harm to breastfed babies) classification as well as a combination of BCF ≥ 100 (and BMF > 1 and log K_{ow} ≥ 3) + R21/R22/R48. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.
- For pentaBDE, no A1 value and no drinking-water standard (DW standard) are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DWS needs to be derived.

4.1.3 Human toxicological threshold limits

In the WFD draft datasheet (Anonymus, 2004), the lowest relevant NOAEL (no observed adverse effect level) is 0.45 $mg.kg_{bw}^{-1}.day^{-1}$ liver toxicity in rats, obtained from a 30 day dietary toxicity study. An AF (assessment factor) of 100 is applied, according to WFD guidance, to derive the TL_{hh}. The NOAEL divided by the AF results in a TL_{hh} of 4.5 $\mu g.kg_{bw}^{-1}.d^{-1}$.

P.M. 1 Note however, that in the EU-RAR an AF of 10000 was applied, consisting of between (factor 10) and within species variation (10), extrapolation from short to long term tests (10), and an extra factor for extrapolation to the population of breast-feeding infants (10). The resulting NOEAL would thus be a factor of 100 lower than the one determined in the draft WFD datasheet.

P.M. 2 Note that the quality standard determined in the datasheet neglects effects on reproduction, which is the most sensitive endpoint. In rodents, lower chlorinated PBDEs may induce developmental toxicity, developmental neurotoxicity and disturbance of homeostasis of thyroid hormones. In a recent report by De Winter-Sorkina *et al*. (2006), a chronic oral threshold value of 0.26 $ng.kg_{bw}^{-1}.d^{-1}$ for pentaBDE nr. 99 (one isomer from the group of pentaBDEs) is derived. This threshold value is based on a LOAEL of 0.06 $mg.kg_{bw}^{-1}.d^{-1}$ from a study in which a single dosage to pregnant rats caused reduced sperm production in male offspring at adulthood, i.e. 140 days *post natum* (Kuriyama *et al.*, 2005). Kinetic properties of PBDEs indicate that these compounds have dioxin-like, bioaccumulating properties in mammals (De Winter-Sorkina *et al.*, 2006). The methodology for derivation of the threshold level was the same as has been applied to the dioxin 2,3,7,8-TCDD, as proposed by JECFA (Joint expert committee on food additives; JECFA (2002) as cited in De Winter *et al*., 2006). The threshold value is derived on the basis of kinetic calculations combined with extrapolation factors.

For the ERL derivation in this report the TL_{hh} of 0.26 $ng.kg_{bw}^{-1}.d^{-1}$ will be used, since the endpoint it is based on is more relevant than that used in the WFD fact sheet.

4.2 p-*tert*-octylphenol

4.2.1 Bioconcentration

Experimentally determined whole fish BCF values for p-*tert*-octylphenol are 261 and 471 $L.kg^{-1}$ and 46-247 $L.kg^{-1}$ for field determined BCFs. A value of 634 $L.kg^{-1}$ is calculated using the QSAR put forward in the TGD. All data from Brooke *et al*. (2005). The latter value was selected as a reasonable worst case by Brooke *et al*. and will be used in calculations presented here.

4.2.2 Trigger values

Table 32. p-tert-octylphenol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	2.43[c]; 2.54 - 3.3[d]	[-]	-	K_{oc} x $f_{oc,\ susp}$
BCF	634	[L.kg^{-1}]	56	TGD QSAR
BMF	2[a]	[-]	-	default values
Log K_{ow}	4.12	[-]	24	shake flask
R-phrases	R50/53, R38[b], 41[b], **62**[b], **63**[b]	[-]	-	
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available
[a]Both BMF_1 and BMF_2 have the value 2, according to the selection table.
[b]Dutch proposal. The Netherlands (RIVM) have proposed R62, R63 (reprotoxic) classification at the TC C&L in March, 2005.
[c]This value is calculated from the selected K_{oc} from Brooke *et al*. (2005), which is also used for calculations in the WFD fact sheet.
[d]The range 2.54 – 3.3 is mentioned in the WFD fact sheet in order to investigate necessity of sediment ERL derivation.

- p-*tert*-octylphenol has a log $K_{p,\ susp\text{-}water} < 3$; when the value of 2.43 is used (as cited by the WFD fact sheet for use of calculations from Brooke *et al*.. For comparison with the sediment trigger, the range of 2.54 – 3.3 is used in the WFD fact sheet. An inconclusive statement was drawn: derivation $MPC_{eco,\ sediment}$ is not triggered, since the trigger was not met, but this was not 'unequivocally'. For INS purposes, an $MPC_{eco,\ sediment}$ will be derived.
- p-*tert*-octylphenol has a (calculated) BCF > 100; assessment of secondary poisoning is triggered.
- p-*tert*-octylphenol has a BCF > 100 plus a potential classification as toxic to reproduction. Although there is no general agreement on the human health classification (see text below) an MPC_{water} for human health via food (fish) consumption will be derived here.
- Since both an A1 value and a DW standard are not available, a provisional drinking-water standard has to be derived.

Agreement on the classification of 4-tert-octylphenol as a 'dangerous substance' for Annex I of Directive 67/548/EEC was reached recently (September 2004), and it is now formally classified as dangerous for the environment (Brooke *et al.*, 2005). According to the ECB, p-*tert*-octylphenol has not been classified in the Annex I of Directive 67/548/EEC, therefore, no further information on classification and labelling information is available (ECB, 2005). Hence, no R-phrases have been set in the framework of EU existing substances, that might trigger risk limit derivation based on human food consumption. The Environment Agency report does not contain a human health classification either (Brooke *et al.*, 2005). p-*tert*-Octylphenol is not listed in the evaluations on carcinogenicity by the IARC (accessed May 29, 2006). The WFD fact sheet refers to a draft version of the report of Brooke *et al*. in which a R48/22 classification was suggested (Anonymus, 2005a). In August 2004, Norway proposed to classify p-*tert*-octylphenol as toxic to reproduction (fertility and developmental toxicity). However, CEPAD, the European Council for Alkylphenols and Derivatives that represents suppliers and users of alkylphenols have opposed against this classification-proposal. To the best of our knowledge, a definitive conclusion on human health classification has not yet been reached. The classification as shown in Table 32 will be used for ERL derivation, meaning that R62, R63 proposals by the Netherlands trigger derivation of $MPC_{water,\ hh\ food}$.

4.2.3 Human toxicological threshold limits

Data in this section are cited from Anonymus (2005a) and Brooke *et al*. (2005).
A NOAEL of 15 $mg.kg_{bw}^{-1}.d^{-1}$ is derived from a 2-generation study on rats (endpoints systemic toxicity and postnatal toxicity). The conversion factor to concentration in food is 20 for rats that are more than 6 weeks old, giving a NOEC (no observed effect concentration) of 300 $mg.kg_{fd}^{-1}$. As the result is derived from a chronic study, the appropriate assessment factor is 30, giving an $MPC_{oral,\ min}$ of 10 $mg.kg_{fd}^{-1}$.

4.3 Benzo[*b*]fluoranthene

4.3.1 Bioconcentration

Water
In the current draft version of the EU-RAR on coal tar pitch (EC, 2006b), no BCF value for benzo[*b*]fluoranthene is available: no experimental data have been found. Using the QSARs mentioned in the TGD, a BCF value of 31768 $L.kg^{-1}$ (Veith QSAR) or 36000 $L.kg^{-1}$ (parabolic QSAR) is estimated. These values are unrealistically high, which will be discussed in the following.
The range of BCF values for fish species reported in the draft EU-RAR for PAHs containing four rings is 200-9054 $L.kg^{-1}$. For the three five ringed PAHs treated in the EU-RAR (one of which is benzo[*b*]fluoranthene), no experimentally determined BCF_{fish} values are available. The EU-RAR postulates that the heavier (molecular weight) PAHs are more rapidly metabolised than the lighter PAHs, due to differences in enzyme activity; however, weight categories were not defined. This suggestion implies lower BCF values for five ring PAHs compared to values reported here for the four ring PAHs.
It is expected that ingestion of sediment by deposit feeding animals may be the dominant route of uptake when hydrophobic compounds have a log K_{ow} > approximately 5.5. The latter finding would also contribute to lower BCF values for most fish species. However, these findings are not corroborated by experimental values for benzo[*b*]fluoranthene.
Higher BCF values are found for lower organisms: BCF values for four ring PAHs for crustaceans range from 180-21916 $L.kg^{-1}$. This corresponds with the knowledge that higher organisms have the ability to biotransform PAH, while lower organisms seem to lack this ability. Mussels seem to have a very limited ability to metabolise PAHs while for algae and oligochaete worms no evidence of PAH metabolism was found. The EU-RAR considers it relevant to incorporate the food chain: water → mollusc → mollusc eating bird/mammal, in the risk assessment.
However, the most recent draft of the EU-RAR does not present a BCF for benzo[*b*]fluoranthene. Since both a BCF and a $PNEC_{oral}$ are missing, risk limits based on secondary poisoning can not be derived.

Soil
Since a $PNEC_{oral}$ has not been derived in the draft EU-RAR, risk limits based on secondary poisoning for soil can not be derived.

4.3.2 Trigger values

Table 33. Benz[b]fluoranthene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	4.91	[-]	58	K_{oc} x $f_{oc,\ susp}$
BCF	n.a.	[L.kg^{-1}]	see section 4.3.1	
BMF	1	[-]	section 4.3.3.1	
Log K_{ow}	6.12	[-]		
R-phrases	R45, 50/53	[-]		
A1 value	0.0002[a]	[mg.L^{-1}]		
DW standard	0.10	[µg.L^{-1}]		

n.a. = not available.
[a]Directive 75/440/EC (EC, 1975) states: polycyclic aromatic hydrocarbons, but does not specify individual compounds.
[b]Directive 98/83/EC (EC, 1998) states that this trigger value stands for the sum of concentrations of 4 PAH, viz. benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene and indeno[1,2,3-cd]pyrene.

- benzo[*b*]fluoranthene has a log $K_{p,\ susp\text{-}water}$ > 3; derivation of $MPC_{eco,\ sediment}$ is triggered.
- benzo[*b*]fluoranthene has a log $K_{p,\ susp\text{-}water}$ > 3; expression of the MPC_{water} as MPC_{water} in suspended particulate matter is required.
- benzo[*b*]fluoranthene has a BCF > 100; assessment of secondary poisoning is triggered.
- benzo[*b*]fluoranthene has an R45 (may cause cancer) classification. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.
- For benzo[*b*]fluoranthene, both an A1 value and a DW standard are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. See section 6.1.3.4 for the use of these standards in ERL derivation.

4.3.3 Secondary poisoning

4.3.3.1 Biomagnification

Although species from lower trophic levels may accumulate PAHs, predators usually contain low levels, a process called biominification. This is due to the possibilities of vertebrates and some invertebrates to excrete and metabolise PAHs. Lower organisms apparently lack the property to metabolise PAHs. The draft EU-RAR concludes that biomagnification of PAHs in food webs at higher trophic levels ‘does not appear to exist’.

In the draft EU-RAR, short attention is given to the possibility of lower organisms to transfer PAHs in the food web, e.g. predatory molluscs and polychaetes might accumulate PAHs. However, due to very limited information, this item is not addressed further, as is the possibility of food web transfer of PAH metabolites.

Based on the information on biominification, a BMF value of 1 is selected for ERL derivation. This decision is in line with the most recent draft of the EU-RAR.

4.3.3.2 Toxicity data on birds and mammals

This section is cited from the draft EU-RAR on coal tar pitch (EC, 2006b). References in the following citation are not included in the reference list.
‘The Technical Guidance Document recommends that the NOAEL from dietary toxicity tests with fish-eating birds or mammals are used to determine the $PNEC_{oral}$. However, data on the PAH toxicity to birds are few. Some pertinent data from the literature are reviewed by Albers and Loughlin (2003): Patton and Dieter (1980) exposed mallards (*Anas platyrhynchos*) to a diet containing 10 PAHs for 7 months and observed greater hepatic stress responses and higher testis

weights than male mallards fed a mixture of 10 alkanes. Retardation of nestling weight gain and increased adrenal and nasal gland weights was attributed to the PAHs with four or more rings. Immune function and MFO activity of European starlings (*Sturnus vulgaris*) were altered by oral or subcutaneous doses of 7,12-dimethylbenzo[*a*]anthracene, a four-ring PAH (Trust *et al*., 1994). From these data it is not possible to derive a NOAEL for birds for either of the PAHs.
Also PAH toxicity data to mammals is limited. Almost all of the long term studies reported were designed to assess carcinogenic potency of PAH and are not considered appropriate for the environmental risk assessment. Only for B[*a*]P reprotoxicity data are available. Most severe effect were observed after administration of 10 $mg.kg^{-1}$ to CD-1 mice by gavage during gestation which produced decreased gonadal weights and reduced fertility and reproductive capacity in the offspring. Higher doses (40 $mg.kg^{-1}$) caused almost complete sterility in both sexes of offspring (Mackenzie and Angevine, 1981). As no lower concentrations are tested a NOAEL can not be determined and consequently no $PNEC_{oral}$ can be derived.
Other mammalian toxicity data for acenaphthene, anthracene, B[*a*]P, fluorene, fluoranthene and pyrene derived from 90 day studies with mice (see Table 34), are based on endpoints which ecological relevance is questionable.'

The conclusion drawn in the most recent draft of the EU-RAR is that derivation of a $PNEC_{oral}$ for benzo[*b*]fluoranthene is not possible. Hence, derivation of an MPC based on secondary poisoning in both soil and water, is not possible.

Table 34. NOAELs for PAHs found in a 90 sub chronic toxicity study with mice taken from IPCS report (WHO, 1998).

Compound	NOAEL [$mg.kg_{bw}^{-1}.d^{-1}$]	Lowest Toxicity endpoint
Acenaphthene	175	Hepatoxicity
Anthracene	1000	No toxicity observed
Benzo[*a*]pyrene	< 1100	Growth
Fluorene	125	Heamatological effect
Fluoranthene	125	Increased ALAT activity, pathological effect in the kidney and liver and clinical and haematological changes
Pyrene	125	Nephropathy and decreased kidney weight

4.3.4 Human toxicological threshold limits

Benzo[*b*]fluoranthene is classified as possibly carcinogenic to humans (see page 28) and has an R45 classification. Baars *et al*. (RIVM, 2001) have derived a maximum permissible risk (MPR) value, which is a CR_{oral} of 5.0 $\mu g.kg_{bw}^{-1}.d^{-1}$. The quality of this risk value is stated as 'high'. CR_{oral} stands for excess lifetime cancer risk via oral exposure. It is based on a lifetime cancer risk of $1:10^4$. As the WFD guidance prefers basing risk limits on a $1:10^6$ lifetime cancer risk, the TL_{hh} is calculated as CR_{oral} /100 = 50 $ng.kg_{bw}^{-1}.d^{-1}$.

4.4 Isodrin

Isodrin was prioritised under the former 'Water Framework Directive' 76/464/EEC (EC, 1976), in the daughter Directive 88/347/EEC (EC, 1988; amending Annex II of 86/280/EC on limit values and quality objectives for discharges of certain dangerous substances included in List I of the Annex to Directive 76/363/EEC). In 88/347/EEC, environmental quality objectives for the sum of aldrin, dieldrin, endrin and isodrin were set at 10 $ng.L^{-1}$ for inland and estuary waters and at 5 $ng.L^{-1}$ for coastal and territorial waters. The European Commission has decided to prioritise isodrin (and several other substances) although the Water Framework Directive 2000/60/EC does not include

isodrin as priority substance but as 'other pollutant'. The environmental quality objectives of 10 and 5 ng.L^{-1} for Σ aldrin, dieldrin, endrin and isodrin are still in force under 2000/60/EC.

For this report we have decided to present only the environmental quality standard for water set in 88/347/EEC under 76/464/EEC and not to derive EQSs for other environmental compartments (see section 3.1.4). Therefore, this section contains no table with trigger values.

4.5 DNOC

4.5.1 Bioconcentration

Since no experimental data on bioconcentration were retrieved for DNOC, a BCF was estimated using the QSAR proposed by the TGD. The calculated BCF is 12.9 L.kg^{-1} indicating that DNOC has no potential to bioaccumulate.

4.5.2 Trigger values

Table 35. DNOC: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	1.25	[-]	32	K_{oc} x $f_{oc,\ susp}$
BCF	12.9	[L.kg^{-1}]	61	TGD QSAR
BMF	–[a]	[-]		
Log K_{ow}	2.13	[-]	30	ClogP (measured)
R-phrases	R 26/27/28, 38, 41, 43, 44, 50/53, 68	[-]		ECB (2000b)
A1 value	1[b]	[µg.L^{-1}]		
DW standard	0.1[c]	[µg.L^{-1}]		

n.a. = not available.
[a]BMF not needed since there is no bioaccumulation potential.
[b]75/440/EC (EC, 1975) states that the sum of total pesticides should not exceed 1 µg.L^{-1}.
[c]not used since an A1 value is available.

- DNOC has a log $K_{p,\ susp\text{-}water}$ < 3; derivation of $MPC_{eco,\ sediment}$ is not triggered.
- No experimental BCF value for DNOC is available. The log K_{ow} of DNOC is < 3, therefore assessment of secondary poisoning is not triggered.
- DNOC has a log K_{ow} < 3 and no relevant R classification; there is no need to derive an $MPC_{hh\ food,\ water}$ for protection of human health via food (fish) consumption.
- An A1 value of 1 µg.L^{-1} for the sum of 'total pesticides[5]' is set. If the other aquatic MPC values derived for DNOC are higher than 1 µg.L^{-1}, the MPC will be set at this value.

4.5.3 Human toxicological threshold limits

ATSDR (Agency for toxic substances and disease registry) has evaluated the non cancer oral toxicity data for DNOC, but did not derive a chronic duration minimal risk level (MRL) because no studies of chronic duration were located. However, ATSDR did derive an intermediate-duration MRL of 0.004 mg.kg_{bw}^{-1}.d^{-1} for neurological effects in a human who took DNOC for the purpose of weight reduction. This MRL will be used as TL_{hh}.

[5] 75/440/EC contains a 1 µg.L^{-1} A1 value for 'Total pesticides (parathion, BHC, dieldrin)'. For the purpose of risk limit derivation, the three pesticides mentioned by name are considered to be examples. The A1 value is interpreted as being valid for the sum of all pesticides measured in a given water body. This wording does not offer possibilities for the setting of A1 values for individual pesticides in the case that more than one pesticide is monitored in a given water body. If only one pesticide is present, its A1 value would be 1 µg.L^{-1}.

4.6 Aniline

4.6.1 Bioconcentration

In the RAR for aniline, it is reported that only one reliable study is available concerning the bioaccumulation of aniline in fish (Zok *et al*., 1991 in EC, 2004a). In this study, *Danio rerio* was exposed to ^{14}C-labelled aniline at a concentration of 0.2 µg.L^{-1} under static conditions. The amount of radioactivity in the medium was kept constant by adding stock solution if required. After reaching a steady state of uptake and elimination, the remaining fish were transferred to a flow-through system containing clean water. A BCF of 2.6 ± 0.06 L.kg^{-1} was determined. This result is in accordance with the measured value for log K_{ow} of 0.9.

4.6.2 Trigger values

Table 36. Aniline: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	1.61	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	2.6[a]	[L.kg^{-1}]	62	flow-through
BMF	–[b]	[-]		
Log K_{ow}	0.9	[-]	34	shake flask
R-phrases	R 23/24/25-40-41-43-48/23/24/25-68-50	[-]		
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]For *Danio rerio* (EC, 2004a).
[b]BMF not needed since there is no bioaccumulation potential.

- Aniline has a log $K_{p,\ susp\text{-}water} < 3$; derivation of $MPC_{eco,\ sediment}$ is not triggered.
- Aniline has a BCF < 100; assessment of secondary poisoning is not triggered.
- Aniline has an R40 (limited evidence of a carcinogenic effect) classification; an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.
- For aniline, no A1 value and no DW standard are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DW standard needs to be derived.

4.6.3 Human toxicological threshold limits

In a repeated dose toxicity study with rats conducted over 104 weeks, a LOAEL of 7.2 mg.kg$_{bw}^{-1}$.d^{-1} was found (CIIT, 1982, cited in EC, 2004a). For the Canadian Environmental Protection Act (Government of Canada, 1994), a TDI has been derived based on the LOAEL of 7.2 mg.kg$_{bw}^{-1}$.d^{-1}. The TDI has been derived by dividing the LOAEL with a factor 5000. The factor of 5000 is the product of factors of 10 for intraspecies variation; 10 for interspecies variation; 10 for use of a LO(A)EL rather than a NO(A)EL and 5 for limited evidence of carcinogenicity. Dividing the LOAEL of 7.2 mg.kg$_{bw}^{-1}$.d^{-1} by 5000 results in a TDI of 1.44 µg.kg$_{bw}^{-1}$.d^{-1}.

This value for the TDI is similar to that which could be derived from the results of the limited clinical study reported by Jenkins *et al*. (1972, cited in EC, 2004a) on formation of methemoglobin in volunteers administered aniline. In derivation of a TDI on the basis of this study in humans, the NOEL (no observed effect level) of 0.21 mg.kg$_{bw}^{-1}$ could be divided by an uncertainty factor of 50 (which takes into account intraspecies variation and limitations of the study), yielding a value of 4.2 µg.kg$_{bw}^{-1}$.d^{-1}.

4.7 Epichlorohydrin

4.7.1 Bioconcentration

For epichlorohydrin (classified with R45), a BCF is needed for calculation of the $MPC_{hh\ food,\ water}$. An experimentally determined bioconcentration factor for epichlorohydrin is not available. Calculation using the QSAR from the TGD (recommended for substances with a log K_{ow} of 2-6) gives a value of -0.318 $L.kg^{-1}$, which is unrealistically low. Using the BCFWIN module from EPI suite, a value of 3.16 $L.kg^{-1}$ is calculated, which will be used as estimate in the calculation of the $MPC_{hh\ food,\ water}$.

4.7.2 Trigger values

Table 37. Epichlorohydrin: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	1.09 [a]	[-]		K_{oc} x $f_{oc,\ susp}$ Anonymus, 2004; EC, 2004a
BCF	3.16	[$L.kg^{-1}$]	63	
BMF	1 [b]	[-]		
Log K_{ow}	0.45	[-]	37	slow-stirring method
R-phrases	R10, R23/24/25, R34, R43, R45	[-]		
A1 value	n.a.			
DW standard	0.1	[$\mu g.L^{-1}$]		

n.a. = not available.
[a]Maximum value calculated with upper limit of K_{oc} range 4.49 – 123.
[b]Default value (INS guidance).

- Epichlorohydrin has a log $K_{p,\ susp\text{-}water} < 3$; even when the upper limit of the available range of K_{oc} values is used. Therefore, derivation of $MPC_{eco,\ sediment}$ is not triggered.
- Epichlorohydrin has a log $K_{ow} < 3$, therefore assessment of secondary poisoning is not triggered.
- Epichlorohydrin is classified as a class 2 carcinogen (class 2A: probable human carcinogen). An MPC_{water} for human health via food (fish) consumption will be derived.
- A DW standard of 0.1 $\mu g.L^{-1}$ is available for epichlorohydrin. If the DW standard is lower than water quality standards for other objectives, a provisional drinking-water standard has to be derived.

4.7.3 Human toxicological threshold limits

The human toxicological threshold limit used for ERL derivation is based on the RSD (risk specific dose) value of 1×10^{-3} $mg.kg_{bw}^{-1}.d^{-1}$, which is based on an oral slope factor and on a $1:10^5$ cancer risk based on lifelong exposure. This RSD is divided by 10 to convert it to a $1:10^6$ cancer risk value. A 10^6 risk value for cancer is in line with the FHI guidance. Therefore, the human risk limit used for ERL derivation in this report, called TL_{hh}, is 0.1 $\mu g.kg_{bw}^{-1}.d^{-1}$.
The RSD value of the US EPA (united states environmental protection agency) is preferred over the TDI of 0.14 $\mu g.kg_{bw}^{-1}.d^{-1}$ published by the World Health Organisation (WHO) (WHO, 2004), since the former value is based on carcinogenicity. Note that the TDI put forward by the WHO and the TL_{hh} used in this report, are highly comparable.

4.8 1,2-Dibromoethane

4.8.1 Bioconcentration

Since 1,2-dibromoethane is carcinogenic, a BCF is needed for $MPC_{hh\ food,\ water}$ derivation. A limited literature search for data on bioconcentration of 1,2-dibromoethane was performed, since bioconcentration was not expected to be relevant for this compound. Mackay *et al*. (2000) reports two calculated BCF values: 6.0 and 2.0 $L.kg^{-1}$. Use of the QSAR put forward in the TGD (and in INS guidance) results in a BCF estimate of 9.25 $L.kg^{-1}$. The applicability domain of this QSAR is log K_{ow} 2-6. With a log K_{ow} of 1.96 we accept this estimate realising that it is a borderline case. BCF estimates are low, which is to be expected based on size of the molecule and its log K_{ow}. In the ERL derivation of 1,2-dibromoethane, the BCF is needed in the ERL derivation for human health via fish consumption ($MPC_{hh\ food,\ water}$). In the absence of experimental BCF data, we propose to calculate the $MPC_{hh\ food,\ water}$ using the highest BCF estimate of 9.25 $L.kg^{-1}$. Further search for experimental BCF values will be performed if the $MPC_{hh\ food,\ water}$ turns out to be the critical MPC_{water}.

4.8.2 Trigger values

Table 38. 1,2-Dibromoethane: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	0.8	[-]		K_{oc} x $f_{oc,\ susp}$
BCF[a]	9.25	[$L.kg^{-1}$]	64	
BMF	-[a]	[-]		
Log K_{ow}	1.96	[-]	39	
R-phrases	R23/24/25, R36/37/38, R45, R51/53	[-]		
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]BMF not needed; BCF < 100 and log K_{ow} < 3.

- Since 1,2 dibromoethane has a log $K_{p,\ susp\text{-}water} < 3$, derivation of $MPC_{eco,\ sediment}$ is not triggered.
- Since 1,2 dibromoethane has a BCF < 100, assessment of secondary poisoning is not triggered.
- Derivation of an MPC_{water} for human health via food (fish) consumption is triggered, since 1,2-dibromoethane is classified as a (suspected) carcinogenic (R45).
- For 1,2-dibromoethane, no A1 value and no DW standard are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DW standard needs to be derived.

4.8.3 Human toxicological threshold limits

1,2-Dibromoethane is classified as a class 2A genotoxic carcinogen by the IARC (Monograph 15, Suppl. 7; IARC, 1999b). A risk specific dose (RSD) of 5.00×10^{-6} $mg.kg_{bw}^{-1}.d^{-1}$ derived by the US EPA, based on a $1:10^5$ risk value for cancer, was retrieved from the TERA (toxicology excellence for risk assessment) database. Based on a $1:10^6$ risk value, this RSD is recalculated to 5.0×10^{-7} $mg.kg_{bw}^{-1}.d^{-1}$. This value will be used as TL_{hh} in ERL derivation.

4.9 Ethinylestradiol

4.9.1 Bioconcentration

There is little information available concerning the bioconcentration potential of ethinylestradiol. Liebig *et al*. (2005) found a BSAF (on a ww/ww basis) of 90 after 35 days in the sediment oligochaete *Lumbriculus variegatus* (lipid content 8 ± 0.4% of dw) although it has to be noted that steady state was not reached. Länge *et al*. (2001) exposed fish (*Pimephales promelas*) to ethinylestradiol for 158 and 245 days and reported that the whole body BCF in healthy fish is likely to be < 500 but certainly below 2400. A more exact determination could not be given due to analytical limitations. Using the QSAR for fish from INS guidance (which is equal to that in the TGD) and a log K_{ow} of 3.67, a BCF value of 263 is calculated. This BCF is used in ERL derivation.

4.9.2 Trigger values

Table 39. Ethinylestradiol: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	2.34[a]	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	263	[L.kg^{-1}]	62	QSAR fish (TGD, 2003)
BMF	1	[-]		Default value; based on log K_{ow}
Log K_{ow}	3.67	[-]	40	Measured
R-phrases	not classified	[-]		ECB, 2005
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]Calculated using log K_{oc} of 3.34 (see section 2.9.3.1).

- Since ethinylestradiol has a log $K_{p,\ susp\text{-}water}$ < 3, derivation of $MPC_{eco,\ sediment}$ is not triggered.
- Since ethinylestradiol has a BCF > 100 (based on the TGD QSAR for fish), assessment of secondary poisoning is triggered.
- Ethinylestradiol has not been classified in Annex I of Directive 67/548/EEC (ECB, 2005), therefore, no R phrases are listed. However, the IARC monograph (IARC, 1979; IARC, 1987b) classifies ethinylestradiol as a class 1 carcinogenic. This triggers derivation of an MPC_{water} for human health via food (fish) consumption.

4.9.3 Human toxicological threshold limits

A human toxicological threshold limit for ethinylestradiol is not available. An ADI for estradiol is available, which is 50 ng.kg$_{bw}^{-1}$.d^{-1} (JECFA, 2000). Ethinylestradiol has a higher estrogenic potency than estradiol. This is caused by the presence of the ethinyl group compared to the estradiol molecule, which causes ethinylestradiol to be much slower metabolised than estradiol. Various values for the difference in estrogenic potency between ethinylestradiol and estradiol in humans are found, none however seems to be very well underpinned. A report by ARCEM (2003) states that the estrogenic potential of ethinylestradiol in humans is 50 times higher than that of estradiol. However, this statement is not referenced. Lobo and Stanczyk (1994) cited a factor of 200 for the difference in potency. After consultation with human toxicologists from RIVM it is proposed to apply a factor of 50 to extrapolate the ADI of estradiol to ethinylestradiol, resulting in a TL_{hh} of 1 ng.kg$_{bw}^{-1}$.d^{-1}. Ethinylestradiol, like other steroidal estrogens, is carcinogenic to humans: IARC Group 1 (IARC, 1979; IARC, 1987b). This carcinogenic action is thought to arise from hormonal receptor-mediated cell growth (non-genotoxic mechanism). Since the ADI protects against hormonal effects it will also be protective against the carcinogenic action by ethinylestradiol.

4.10 Methyl bromide

4.10.1 Bioconcentration

A literature search for experimental data on bioconcentration of methyl bromide was not performed, since bioconcentration is not expected to be relevant for methyl bromide. Mackay *et al*. (2000) reports two calculated BCF values: 0.623 and 0.672 $L.kg^{-1}$. The QSAR put forward in the TGD (and in INS guidance) is not applicable (applicability domain of log K_{ow} 2-6) to methyl bromide. The EPI Suite estimate is 0.206. In the absence of experimental BCF data, we propose to calculate the $MPC_{hh\ food,\ water}$ using the highest BCF estimate of 0.672 $L.kg^{-1}$.

4.10.2 Trigger values

Table 40. Methyl bromide: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	-0.39[a]	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	0.672		66	
BMF	1	[-]		
Log K_{ow}	1.19	[-]	43	
R-phrases	R23/25, R36/37/38, R48/20; R50; R59; R68	[-]		Classification from Annex I under 67/548/EEC.
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]Based on a geometric mean log K_{oc} of 0.606 (see Table 24).

- Since methyl bromide has a log $K_{p,\ susp\text{-}water} < 3$, derivation of $MPC_{eco,\ sediment}$ is not triggered.
- Since methyl bromide has a BCF < 100, assessment of secondary poisoning is not triggered.
- Although methyl bromide is classified with R21 and R48, this does not trigger derivation of an $MPC_{hh\ food,\ water}$ derivation (protection of human health via food (fish) consumption) since methyl bromide does not have the potential to bioaccumulate.
- For methyl bromide, no A1 value and no DW standard are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DW standard needs to be derived.

4.10.3 Human toxicological threshold limits

IARC monograph Vol. 71 concludes the following: 'There is inadequate evidence in humans for the carcinogenicity of methyl bromide. There is limited evidence in experimental animals for the carcinogenicity of methyl bromide. The overall evaluation methyl bromide is not classifiable as to its carcinogenicity to humans (Group 3)' (IARC, 1999a).

ATSDR (ATSDR, 1992) has evaluated the oral toxicity data for methyl bromide, but did not derive a chronic duration minimal risk level (MRL) because no studies of chronic duration were available. However, ATSDR did derive an intermediate-duration MRL of 0.003 $mg.kg_{bw}^{-1}.d^{-1}$. US EPA reports an RfD (reference dose) of 1.40×10^{-3} $mg.kg_{bw}^{-1}.d^{-1}$ (US EPA, 2007a). This RfD is derived from a NOAEL of 1.4 $mg.kg_{bw}^{-1}.d^{-1}$ for epithelial hyperplasia of the fore stomach and an assessment factor of 1000. The RfD of 1.40×10^{-3} $mg.kg_{bw}^{-1}.d^{-1}$ will be used as TL_{hh} in the derivation of the $MPC_{dw,\ water}$.

4.11 6PPD

4.11.1 Bioconcentration

No bioaccumulation studies are available for 6PPD. Based on its calculated log K_{ow} of 5.41, a BCF of 7900 L.kg^{-1} would be calculated using the QSAR recommended in the TGD. However, since 6PPD is not stable in water, as discussed in section 0, it is not expected to bioaccumulate. Experimentally determined BCF values for 6PPD degradation products are maximally 23 for 1,2-dimethylbutylamine and N-phenyl-p-benzoquinone monimine, indicating that there is no bioaccumulation potential for these metabolites (cited from OECD, 2004).

4.11.2 Trigger values

Table 41. 6-PPD: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	3.48[a]	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	<100	[L.kg^{-1}]	67	
BMF	n.a.	[-]		
Log K_{ow}	5.41	[-]	45	ClogP estimate
R-phrases	R43[b], R50[b], R53[b]	[-]		BUA (1998)
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]Based on log K_{oc} of 4.48 (see page 45).
[b]The R phrases have been cited from BUA (1998). To date, 6PPD is not classified in the Annex I of Directive 67/548/EEC. Therefore, the R-phrases should be regarded as indicative.

- Since 6PPD has a log $K_{p,\ susp\text{-}water} \geq 3$, derivation of $MPC_{eco,\ sediment}$ is triggered.
- Since 6PPD has a BCF < 100, assessment of secondary poisoning is not triggered.
- Derivation of an $MPC_{hh\ food,\ water}$ (protection of human health via food (fish) consumption) is not triggered, since 6PPD is not classified as a (suspected) carcinogenic, mutagenic or reprotoxic substance.
- No A1 value and no DW standard are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DWS needs to be derived.

4.11.3 Human toxicological threshold limits

Both OECD (2004) and OSPAR (2005) report 6PPD as a substance which is not carcinogenic, mutagenic and/or reprotoxic (CMR). No established ADI or TDI was found for 6PPD. The NOAEL of 75 mg.kg$_{bw}^{-1}$.d^{-1} reported in the OECD SIDS report is selected as TL_{hh} (OECD, 2004). This NOAEL is based on feeding studies ranging from 13 weeks to 24 months exposure in both male and female rats. Following INS guidance, TL_{hh} is equal to the NOAEL/100, which gives a TL_{hh} of 0.75 mg.kg$_{bw}^{-1}$.d^{-1}.

4.12 DCB

4.12.1 Bioconcentration

For the five bioconcentration studies for fish reported in the IUCLID dataset, the original papers were retrieved and evaluated (Sikka *et al.*, 1978; Appleton and Sikka, 1980; Freitag *et al.*, 1985). The BCF study of Appleton and Sikka was performed at 5 and 0.1 µg.L^{-1}. These concentrations are

far below the LC50 of DCB for *L. macrochirus* (LC50 = 500 µg.L^{-1}). Mortality will not have influenced the determination of BCFs from the study by Appleton and Sikka.
The BCFs from the study by Sikka *et al*. are considered less valid. Mortality of fish at the end of the exposure period hampered determination of equilibrium BCFs. The first experiment showed mortality at an exposure concentration of 2 mg.L^{-1} at the end of the 48 hour exposure period. In the second experiment, the exposure concentration was 0.5 mg.L^{-1} and mortality started to occur after 96 hours of exposure. The authors indicate that equilibrium was not yet reached, given the fact that residues in fish surviving at 120 hours were substantially higher than levels in fish dead at 120 hours and also higher than levels in fish living at 96 hours. Although the higher BCF of the two (554 L.kg^{-1}) is in the same range as the values of Appleton and Sikka, both values were excluded because of the occurrence of mortality of test organisms.
The study of Freitag *et al*. reports a BCF of 610 L.kg^{-1}. However, since this study lacks all experimental detail, it will not be used for ERL derivation. The geometric mean of the two BCF values from Appleton and Sikka is 501 L.kg^{-1}, and this value will be used for ERL derivation.

Preliminary evidence for metabolism of DCB in fish was also obtained in the study by Appleton and Sikka (1980) and Sikka *et al*. (1978) The presence of one metabolite was shown, the identity of which was not elucidated. Preliminary research suggested that this might be a DCB-glucoronide conjugate.
Calculation of the BCF using the QSAR suggested in the TGD, with the selected log K_{ow} of 3.51, gives a BCF of 192 L.kg^{-1}. Since experimental data indicate higher accumulation,
the **BCF of 501** L.kg^{-1}, based on total ^{14}C radioactivity in whole fish is used for ERL derivation.

4.12.2 Trigger values

Table 42. 3,3'-Dichlorobenzidine (DCB): collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method/source (if applicable)
Log $K_{p,\ susp\text{-}water}$	2.99[a]	[-]		K_{oc} x $f_{oc,\ susp}$
BCF	501	[L.kg^{-1}]	67	
BMF	1	[-]		
Log K_{ow}	3.51	[-]	48	measured
R-phrases	R21, R43, R45, R50/53	[-]		ECB (2000b)
A1 value	n.a.			
DW standard	n.a.			

n.a. = not available.
[a]Based on the selected value for log K_{oc} of 3.99.

- The actual value of the log $K_{p,\ susp\text{-}water}$ is < 3. This means that $MPC_{eco,\ sediment}$ derivation would not be triggered. However, rounding off the log $K_{p,\ susp\text{-}water}$ value of 2.99 would give 3, triggering $MPC_{eco,\ sediment}$ derivation. Moreover, since adsorption studies on sediment have shown that part of the sorption of DCB to sediment is irreversible, it is reasonable to expect that sediment concentrations will slightly increase over the values estimated with equilibrium partitioning. It was therefore decided to derive an $MPC_{eco,\ sediment}$ for DCB.
- Since DCB has a BCF > 100, assessment of secondary poisoning is triggered.
- Derivation of an MPC_{water} for human health via food (fish) consumption is triggered, since DCB is classified as a (suspected) carcinogen, and its BCF ≥ 100 is coupled to R21.
- No A1 value and no DWS are available from Council Directives 75/440/EEC (EC, 1975) and 98/83/EC (EC, 1998), respectively. Therefore, a provisional DWS needs to be derived.

4.12.3 Human toxicological threshold limits

Epidemiological studies have shown that benzidine induces urinary bladder cancer in workers in the azo-dye industry. In animals, other target organs for carcinogenesis caused by aromatic amines have been identified, depending on the exposure route (Zeilmaker *et al.*, 2000).
Zeilmaker *et al*. have derived an NRL (negligible risk level) for DCB was derived from the NRL for benzidine, which is 0.3 $ng.d^{-1}$. This value is based on benzidine levels in urine of exposed workers, oral benzidine exposure and urinary excretion in rhesus monkeys and an extrapolation model.
A correction factor of 10 was applied by Zeilmaker *et al*. to account for the difference in carcinogenic potency between benzidine and DCB. This correction factor is a conservative estimate based on the difference in carcinogenic potency (TD50) values of benzidine and DCB, which were reported to be 1.7 $mg.kg_{bw}^{-1}.d^{-1}$ and 28 $mg.kg_{bw}^{-1}.d^{-1}$, respectively. Hence, the NRL for DCB is 3 $ng.d^{-1}$. This NRL is based on life long exposure leading to 1 extra case of cancer in one million life-long exposed persons. The NRL is equal to 3/70 = 0.043 $ng.kg_{bw}^{-1}.d^{-1}$. The latter value will be used as TL_{hh} in the ERL derivation.

4.12.4 Secondary poisoning

An online literature search in TOXLINE (1985-2001) and CURRENT CONTENTS (1997-June 2006) was performed to find studies on birds and mammals that would result in NOEC, NOEL or NOAEL levels of DCB toxicity. Surprisingly, no studies on bird toxicity of DCB were retrieved, nor were any studies with DCB resulting in a NOEC, NOEL or a NOAEL found.
Several other sources were screened for bird and (chronic) mammal toxicity studies: GDCh (German Chemical Society)-BUA (1989), GDCh (German Chemical Society)-BUA (1999), Government of Canada (1993), ECB (2000b); but no NOAELs or useful studies were reported. In ATSDR (1998), the available study information on oral toxicity of DCB to mammals is summarised and represented as NOAELs. The lowest NOAEL reported for chronic exposure is 10 $mg.kg_{bw}^{-1}.d^{-1}$ obtained in a seven year study with dogs. However, the lowest LOAELs reported, are approximately 11 $mg.kg_{bw}^{-1}.d^{-1}$ for incidence of hepatic tumours in mice and 10.4 $mg.kg_{bw}^{-1}.d^{-1}$ for hepatocellular and urinary bladder carcinomas in dogs. Note however, that these LOAELs can not be considered valid, since in both studies only one dose was tested. Summarising, this means that there are not enough data to derive a robust NOAEL for birds or mammals.
We propose, pragmatically, to divide the NOAEL of 10 $mg.kg_{bw}^{-1}.d^{-1}$ obtained for dogs, by an assessment factor of 10, and to use the resulting extrapolated NOAEL of 1 $mg.kg_{bw}^{-1}.d^{-1}$, as input for the derivation of an MPC for secondary poisoning. This NOAEL of 1 $mg.kg_{bw}^{-1}.d^{-1}$ is converted to a $NOEC_{mammal}$ using a conversion factor of 40 $g_{bw}.g_{fd}^{-1}.d^{-1}$ for food intake, resulting in a $NOEC_{mammal\ food\ chr}$ of 40 $mg.kg_{fd}^{-1}$.

5. *Ad hoc*-MPC values and underlying data

5.1 Overview of a*d hoc*-MPCs for water

Table 43 presents *ad hoc*-MPC values for the compartment water for the twelve substances investigated in this report. The following sections show the toxicity data underlying these *ad hoc*-MPCs, for those cases where the data could be retrieved.

Table 43. Ad hoc-MPC values derived by RIZA[h] and RIVM[i] for 12 selected substances.

Compound	*ad hoc*-MPC RIZA [µg.L^{-1}]	Reference	*ad hoc*-MPC RIVM [µg.L^{-1}]	Reference
pentaBDE	0.014	Anonymus, 2006a, Anonymus, 2006b	0.53[e]	see footnote e
p-*tert*-octylphenol	0.122; 3.2[a]	Anonymus, 2006a, Anonymus, 2006b	0.00423	Hansler and Posthumus, in prep.
benzo[*b*]fluoranthene	0.025[b]	see footnote b	0.024[e]	see footnote e
isodrin	0.008	Beek, 1999	0.00082	Hansler and Posthumus, in prep.
DNOC	196, 21[c]	Beek, 1999	–[f]	Hansler and Posthumus, in prep.
aniline	0.08	Anonymus, 2006a, Anonymus, 2006b	0.4[e]	Hansler and Posthumus, in prep.
epichlorohydrin	12	Beek, 2002	2.95	Hansler and Posthumus, in prep.
1,2-dibromoethane	4.8	Beek, 2002	5.96×10^{-5} [g]	Hansler and Posthumus, in prep.
ethinylestradiol	1	Anonymus, 2006a, Anonymus, 2006b	0.189	Hansler and Posthumus, in prep.
methyl bromide	7000[d]; 7[d]	Beek, 1999	0.42	Hansler and Posthumus, in prep.
6PPD	2.4	Anonymus, 2006a, Anonymus, 2006b	0.0538	Hansler and Posthumus, in prep.
3,3'-dichlorobenzidine	1	Beek, 2002	0.000256	Hansler and Posthumus, in prep.

[a]The value of 0.122 µg.L^{-1} was reported in Anonymus, 2006a and Anonymus, 2006b, while Hansler and Posthumus (in prep.) report an *ad hoc*-MPC derived by RIZA of 3.2 µg.L^{-1}.
[b]RIZA did not derive an *ad hoc*-MPC benzo[*b*]fluoranthene in Beek, 2002. In that report, a German standard (QZ, qualitätsziel, 'quality standard') of 0.025 µg.L^{-1} is cited. Most likely, this value was used to set the *ad hoc*-MPC published as 'MKN' value of 0.025 µg.L^{-1}; see also section 5.2.3.
[c]RIZA has derived two *ad hoc*-MPC values for DNOC: one tabulated as 2-methyl-4,6-dinitrophenol, the other tabulated as DNOC.
[d]RIZA has published two *ad hoc*-MPC values for methyl bromide: one tabulated as 7 mg.L^{-1} (Anonymus, 2006a) and one as 7 µg.L^{-1} (Beek, 1999;Anonymus, 2006b).
[e]The value reported in the table was used to prioritise the twelve compounds for this project, but stems from an earlier draft of Hansler and Posthumus. In a later version of Hansler and Posthumus (in prep.), cited here, the proposed *ad hoc*-MPC was removed, since a since a draft EU-RAR exists for this compound.
[f]No *ad hoc*-MPCs derived by RIVM for DNOC since an MPC value (21 µg.L^{-1}) already existed (see section 5.2.5).
[g]This value was proposed in the first draft of Hansler and Posthumus and it was used to prioritise 1,2-dibromoethane for ERL derivation. In a later version of Hansler and Posthumus (in prep.), the proposed *ad hoc*-MPC was removed, since a legally binding MPC value already existed (see section 5.3.2).
[h]RIZA = institute for inland water management and waste water treatment.
[i]RIVM = national institute for public health and the environment.

5.2 GROUP 1: compounds for which ERL derivation is ongoing in various frameworks

5.2.1 PentaBDE

- An *ad hoc*-MPC for pentaBDE has not been derived by RIVM and awaits finalisation of the EU-RAR for this substance group (Hansler and Posthumus, in prep.).
- The *ad hoc*-MPC derived by RIZA for pentaBDE is 0.014 µg.L^{-1} (Anonymus, 2006b; Anonymus, 2006a). This value expresses the dissolved fraction.

5.2.2 p-*tert*-octylphenol

- The *ad hoc*-MPC for p-*tert*-octylphenol derived by RIVM is 0.00423 µg.L^{-1} (Hansler and Posthumus, in prep.). Table 44 shows the toxicity value that was used to derive the RIVM *ad hoc*-MPC.

Table 44. Toxicity datum underlying the RIVM ad hoc-MPC for p-tert-octylphenol.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Selenastrum capricornutum	algae	96 h	EC50	1.9	HSDB

References

HSDB, Hazardous Substances Database, US National Library of Medicine (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB).

The toxicity study listed in Table 44 has been tabulated for ERL derivation in the p-*tert*-octylphenol toxicity data tables (Table A5. 2).

- The *ad hoc*-MPC for p-*tert*-octylphenol derived by RIZA is 0.122 µg.L^{-1} (Anonymus, 2006b; Anonymus, 2006a). This value expresses the dissolved concentration.

5.2.3 Benzo[*b*]fluoranthene

- An *ad hoc*-MPC for benzo[*b*]fluoranthene has not been derived by RIVM and awaits finalisation of the EU-RAR for coal tar pitch (Hansler and Posthumus, in prep.).
- RIZA presents an 'MKN', which is to be interpreted as *ad hoc*-MPC of 0.025 µg.L^{-1} (this value expresses the total concentration, i.e. dissolved + adsorbed to suspended matter) under 76/464/EEC for benzo[*b*]fluoranthene (called 3,4-benzofluoranthene) (Anonymus, 2006b; Anonymus, 2006a).

The derivation of an *ad hoc*-MPC for this compound could not be found. In Beek (2002), one toxicity study is reported, but an *ad hoc*-MPC was not derived. The toxicity datum cited from Beek is given in Table 45.

Table 45. Toxicity datum of benzo[b]fluoranthene cited in RIZA ad hoc-MPC derivation.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Daphnia magna	crustacea	24 h	EC50	>1.024	n.r.

n.r. = not reported.

5.2.4 Isodrin

- The *ad hoc*-MPC for isodrin derived by RIVM is 0.82 ng.L^{-1} (Hansler and Posthumus, in prep.). This report states that this MPC is based on an LC50 value of 6 µg.L^{-1}, but no further details are given.
- RIZA presents a legal MPC of 8 µg.L^{-1} (this value expresses the dissolved fraction) for isodrin, derived under 76/464/EEC (Anonymus, 2006b; Anonymus, 2006a).

An *ad hoc*-MPC for isodrin derived by RIZA was reported by Beek (Beek, 1999), this value is 8 ng.L^{-1} (Phernambucq *et al.*, 1996).

5.2.5 DNOC

- RIVM has not derived an *ad hoc*-MPC value for DNOC since an MPC value for water was available (Hansler and Posthumus, in prep.). This MPC_{water} is 21 µg.L^{-1} (Crommentuijn *et al.*, 1997).
- RIZA also presents an MPC (not an *ad hoc*-MPC) for DNOC of 21 µg.L^{-1} (Anonymus, 2006b; Anonymus, 2006a). The MPC values for the total and dissolved fraction of DNOC are equal. RIZA has earlier reported an *ad hoc*-MPC value of 196 µg.L^{-1} for 2-methyl-4,6-dinitrophenol (Beek, 1999), while in the same report and table an *ad hoc*-MPC of 21 µg.L^{-1} is reported for DNOC. Presumably, the identity of DNOC (dinitro-*ortho*-cresol), being 2-methyl-4,6-

dinitrophenol, was overlooked. However, the underlying toxicity data for both *ad hoc*-MPCs is not presented.

5.2.6 Aniline

- An *ad hoc*-MPC for aniline has not been derived by RIVM and awaits finalisation of the EU-RAR for this substance (Hansler and Posthumus, in prep.).
- The *ad hoc*-MPC derived by RIZA for aniline is 0.08 $\mu g.L^{-1}$ (Anonymus, 2006b; Anonymus, 2006a). This value expresses the dissolved fraction.

5.3 GROUP 2: compounds for which only *ad hoc*-MPCs are available

5.3.1 Epichlorohydrin

- The *ad hoc*-MPC for epichlorohydrin derived by RIVM is 2.95 $\mu g.L^{-1}$ (Hansler and Posthumus, in prep.). Table 46 shows the toxicity data that were used to derive the RIVM *ad hoc*-MPC.

Table 46. Toxicity data underlying the RIVM ad hoc-MPC for epichlorohydrin.

Species	Taxon	Duration	Criterion	Value [$mg.L^{-1}$]	Reference
Microcystis aeruginosa	bacteria	8 d	NOEC	6	IUCLID
Chilomonas paramaecium	protozoa	48 h	NOEC	29	IUCLID
Scenedesmus quadricauda	algae	8 d	NOEC	5.4	IUCLID
Daphnia magna	crustacea	48 h	LC50	19.4*	ECOTOX
Pimephales promelas	pisces	96 h	LC50	9.1*	ECOTOX

*this value is the lower limit of an LC50 range.

References

IUCLID, International Uniform Chemical Information system (http://ecb.jrc.it/existing-chemicals/).

ECOTOX, Aquatic toxicity database van US EPA (http://www.epa.gov/cgi-bin/ecotox_quick_search).

The majority of values listed in Table 46 have been tabulated for ERL derivation in the epichlorohydrin toxicity data tables. Some data could not be identified due to the omission of original references.

- RIZA presents a legal MPC (NB not an *ad hoc*-MPC) for epichlorohydrin of 12 $\mu g.L^{-1}$ (dissolved fraction), derived under 76/464/EEC (Anonymus, 2006b; Anonymus, 2006a). This MPC was derived as *ad hoc*-MPC in Beek (2002). The toxicity data used in this derivation and cited from that report are listed in Table 47. All toxicity tests used for the RIZA *ad hoc*-MPC derivation are tabulated for the MPC derivation in this report.

Table 47. Toxicity data underlying the RIZA ad hoc-MPC for epichlorohydrin.

Species	Taxon	Duration	Criterion	Value [$mg.L^{-1}$]	Reference
Daphnia magna	crustacea	48 h	LC50	24	n.r.
Carassius auratus	pisces	24 h	LC50	23	n.r.
Danio rerio	pisces	96 h	LC50	30.5	n.r.
Lepomis macrochirus	pisces	96 h	LC50	35	n.r.
Menidia beryllina	pisces (marine)	96 h	LC50	18	n.r.
Pimephales promelas	pisces	96 h	LC50	12	n.r.
Rasbora heteromorpha	pisces	48 h	CL50	36	n.r.

n.r. = not reported.

Based on the combination of species name and LC50 value, we infer that the majority of values listed in Table 47 have been tabulated for ERL derivation in the epichlorohydrin toxicity data tables. Some data could not be identified due to missing references.

5.3.2 1,2-Dibromoethane

- RIVM has not derived an *ad hoc*-MPC value for 1,2-dibromoethane since there is a legal value according to the 'Scheldt decree' (in Dutch: 'Schelde arrest'; Hansler and Posthumus, in prep.). The height of this value was 4.8 µg.L^{-1} (Anonymus, 2003). However, note that this value is currently no longer in force. Although an *ad hoc*-MPC was not derived by Hansler and Posthumus, the following toxicity data were collected (Table 48).

Table 48. Toxicity data underlying the RIVM ad hoc-MPC for 1,2-dibromoethane.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Hydra oligactis	coelenterata	72 h	LC50	50	ECOTOX
Cyprinodon variegatus	pisces (marine)	48 h	LC50	4.8	ECOTOX
Oryzias latipes	pisces	96 h	NOEC	5.8	ECOTOX

References

ECOTOX, Aquatic toxicity database of US EPA (http://www.epa.gov/cgi-bin/ecotox_quick_search).

All values listed in Table 48 have been tabulated for ERL derivation in the 1,2-dibromoethane toxicity data tables (Table A5. 8, Table A5. 16 and Table A5. 26).

- RIZA presents a legal MPC (NB not an *ad hoc*-MPC) for 1,2-dibromoethane of 4.8 µg.L^{-1} (dissolved fraction), derived under 76/464/EEC (Anonymus, 2006b; Anonymus, 2006a). This MPC was derived as *ad hoc*-MPC in Beek (2002). The toxicity data used in this derivation and cited from that report are listed in Table 49.

Table 49. Toxicity data underlying the RIZA ad hoc-MPC for 1,2-dibromoethane.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Hydra oligactis	coelenterata	72 h	LC50	50	n.r.
Daphnia magna	crustacea	24 h	EC50	55	n.r.
Centropus undecimalis	pisces (marine)	48 h	LC50	6.2	n.r.
Cyprinodon variegatus	pisces (marine)	48 h	LC50	4.8	n.r.
Lepomis macrochirus	pisces	48 h	LC50	21	n.r.
Micropterus salmoides	pisces	48 h	LC50	18	n.r.
Oryzias latipes	pisces	96 h	LC50	32.1	n.r.
Oryzias latipes	pisces	28 d	NOEC	3.74	n.r.

n.r. = not reported.

The majority of values listed in Table 49 have been tabulated for ERL derivation in the 1,2-dibromoethane toxicity data tables. One toxicity datum could not be identified due to the omission of original references (Table A5. 8, Table A5. 16 and Table A5. 26).

5.3.3 Ethinylestradiol

- The *ad hoc*-MPC for ethinylestradiol derived by RIVM is 0.189 µg.L^{-1} (Hansler and Posthumus, in prep.). Although the method of derivation of this *ad hoc*-MPC value, following Hansler and Posthumus, is untraceable, the following toxicity data were collected (Table 50).

Table 50. Toxicity data underlying the RIVM ad hoc-MPC for ethinylestradiol.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Remark	Reference
Hydra vulgaris	coelenterata	96 h	LC50	3.8		Pascoe *et al.*, 2002
Brachionus calyciflorus	rotifera	72 h	EC50	1.33[a]		Radix *et al.*, 2002
Acartia tonsa	crustacea (marine)	5 d	EC50	0.088	development	Andersen *et al.*, 2001
Cyprinodon variegatus	pisces (marine)	73 d	NOEC	0.000017	reproduction	Zillioux *et al.*, 2001
Oryzias latipes	pisces	21 d	NOEC	0.00026	reproduction	Seki *et al.*, 2002
Pimephales promelas (eggs)	pisces	172 d	NOEC	0.0000028	growth	Länge *et al.*, 2001

[a]This value is actually 1.23 mg.L^{-1} when recalculated from the original paper and is used as such in ERL derivation.

All studies listed in Table 50 have been tabulated for ERL derivation in the ethinylestradiol toxicity data tables (Table A5. 9, Table A5. 17 and Table A5. 27). Due to re-evaluation of the studies, differences in listed endpoints and values may occur between Table 50 and the values used in the underlying report.

- The *ad hoc*-MPC derived by RIZA for ethinylestradiol is 1 $\mu g.L^{-1}$ (Anonymus, 2006b; Anonymus, 2006a).

5.3.4 Methyl bromide

- The *ad hoc*-MPC for methyl bromide derived by RIVM is 0.42 $\mu g.L^{-1}$ (Hansler and Posthumus, in prep.). The following toxicity data were collected (Table 51):

Table 51. Toxicity data underlying the RIVM ad hoc-MPC for methyl bromide.

Species	Taxon	Duration	Criterion	Value [$mg.L^{-1}$]	Reference
Chlorella pyrenoidosa	algae	48 h	EC50	5	IUCLID
Scenedesmus quadricauda	algae	48 h	EC50	3.2	IUCLID
Daphnia magna	crustacea	48 h	EC50	2	IUCLID
Menidia beryllina	pisces	96 h	LC50	11	DOSE
Oryzias latipes	pisces	96 h	LC50	0.7	IUCLID
Oryzias latipes	pisces	3 mo	NOEC	0.32	IUCLID
Poecilia reticulata	pisces	72 h	NOEC	0.1	IUCLID

References

IUCLID, International Uniform Chemical Information system (http://ecb.jrc.it/existing-chemicals/).
DOSE- Dictionaire of Substances and their Effects. The Royal Society of Chemistry (CD-ROM).

All studies listed in Table 51, except the study with *M. beryllina*, have been tabulated for ERL derivation in the ethinylestradiol toxicity data tables (Table A5. 10, Table A5. 28). The study with *M. beryllina* could not be retrieved since a reference to the study was missing.

- Two *ad hoc*-MPC values are published by RIZA for methyl bromide: 7 $\mu g.L^{-1}$ (Beek, 1999;Anonymus, 2006b) and 7 $mg.L^{-1}$ (Anonymus, 2006a). Both values express the dissolved fraction of the methyl bromide concentration.

5.3.5 6PPD

- The *ad hoc*-MPC for 6PPD derived by RIVM is 0.0538 $\mu g.L^{-1}$ (Hansler and Posthumus, in prep.). The following toxicity data were collected (Table 52):

Table 52. Toxicity data underlying the RIVM ad hoc-MPC for 6PPD.

Species	Taxon	Duration	Criterion	Value [$mg.L^{-1}$]	Reference
Pseudokirchneriella subcapitata	algae	96 h	EC50	0.6	IUCLID
Daphnia magna	crustacea	48h	EC50	0.51	IUCLID
Lepomis macrochirus	pisces	96 h	LC50	0.4	IUCLID
Oncorhynchus mykiss	pisces	96 h	LC50	0.14	IUCLID
Pimephales promelas	pisces	6 d	LC50	0.35	IUCLID

References

IUCLID, International Uniform Chemical Information system (http://ecb.jrc.it/existing-chemicals/).

Of the toxicity data shown in Table 52, the data for *P. subcapitata* and *D. magna* have been tabulated for ERL derivation in the 6PPD toxicity data tables (Table A5. 11). The toxicity data for fish in Table 52 could not be retrieved.

- The *ad hoc*-MPC derived by RIZA for 6PPD is 2.4 $\mu g.L^{-1}$ (Anonymus, 2006b; Anonymus, 2006a). This values express the dissolved fraction.

5.3.6 DCB

- The *ad hoc*-MPC for DCB derived by RIVM is 0.256 ng.L^{-1} (Hansler and Posthumus, in prep.). The following toxicity data were collected (Table 53).

Table 53. Toxicity data underlying the RIVM ad hoc-MPC for 3,3'-dichlorobenzidine.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Vibrio fischeri	bacteria	15 min	LC50	0.048	IUCLID
Vibrio fischeri	bacteria	15 min	LC50	0.061	DOSE
Scenedesmus subspicatus	algae	72 h	EC50	2.1	IUCLID
Scenedesmus subspicatus	algae	72 h	NOEC	0.32	IUCLID
Daphnia magna	crustacea	48 h	EC50	1.05	ECOTOX
Brachydanio rerio	pisces	96 h	LC50	3.3	IUCLID
Lepomis macrochirus	pisces	120 h	LC50	0.5	IUCLID
Pimephales promelas	pisces	96 h	LC50	1.05	ECOTOX

References
DOSE- Dictionaire of Substances and their Effects. The Royal Society of Chemistry (CD-ROM).
IUCLID, International Uniform Chemical Information system (http://ecb.jrc.it/existing-chemicals/).
ECOTOX, Aquatic toxicity database van US EPA (http://www.epa.gov/cgi-bin/ecotox_quick_search).

The majority of values listed in Table 53 have been tabulated for ERL derivation in the DCB toxicity data tables (Table A5. 12, Table A5. 18). Re-evaluation of studies may cause differences in some of the toxicity values (see 'Remarks' below). One study with *Vibrio fischeri* (EC50 of 0.061 mg.L^{-1}) could not be retrieved due to omission of original references.

Remarks
The value of 0.048 mg.L^{-1} for *V. fischeri* is erroneously cited from IUCLID (ECB, 2000b). The value is actually 0.058 mg.L^{-1}, which is confirmed in the original reference (Dutka and Kwan, 1981).
The value of 2.1 mg.L^{-1} for *S. subspicatus* is for the parameter biomass, while we have selected the value for growth rate (4.3 mg.L^{-1}) from the same experiment[6].

- RIZA presents a legal MPC (NB not an *ad hoc*-MPC) for DCB of 1 µg.L^{-1} (dissolved fraction), derived under 76/464 EEC (Anonymus, 2006b; Anonymus, 2006a).
  This value was derived as *ad hoc*-MPC in Beek (2002). The toxicity data used in this derivation and cited from that report are listed in Table 54.

Table 54. Toxicity data underlying the RIZA ad hoc-MPC for DCB.

Species	Taxon	Duration	Criterion	Value [mg.L^{-1}]	Reference
Daphnia magna	crustacea	48 h	EC50	1.05	n.r.
Pimephales promelas	pisces	96 h	LC50	2.026	n.r.

n.r. = not reported.

One value (EC50 for *D. magna*) listed in Table 47 is also tabulated for ERL derivation in the DCB toxicity data Table A5. 12. The LC50 for *P. promelas* could not be identified due to missing references, but might be one of the values reported by Brooke (1991).

[6] Preference for selection of this endpoint over biomass has been explained in INS guidance.

5.4 *Ad hoc*-MPCs for soil

Ad hoc-MPC values for soil have been derived only by RIVM, not by RIZA. The available information on *ad hoc*-MPC values for soil is summarised in Table 55. Since all presented *ad hoc*-MPC values for soil have been derived using EqP theory, no experimental toxicity data are available.

Table 55. Ad hoc-MPC_{soil} values derived by RIVM for 12 selected substances.

Compound	*ad hoc*-MPC_{soil} [µg.kg^{-1}]	Reference	Method	K_p [L.kg^{-1}]	log K_{oc} [-]
PentaBDE	–[a]	Hansler and Posthumus, in prep.			
p-*tert*-octylphenol	1	Hansler and Posthumus, in prep.	EqP	990	4.23
Benzo[*b*]fluoranthene	–[a]	Hansler and Posthumus, in prep.			
Isodrin	4.29	Hansler and Posthumus, in prep.	EqP	1076	4.26
DNOC	–[b]	Hansler and Posthumus, in prep.			
Aniline	–[a]	Hansler and Posthumus, in prep.			
Epichlorohydrin	0.43	Hansler and Posthumus, in prep.	EqP	1.06	1.25
1,2-dibromoethane	1.98E-05	Hansler and Posthumus, in prep.	EqP	3.71	1.80
Ethinylestradiol	7.3	Hansler and Posthumus, in prep.	EqP	95.8	3.21
Methyl bromide	0.059	Hansler and Posthumus, in prep.	EqP	2.56	1.64
6PPD	0.39	Hansler and Posthumus, in prep.	EqP	366	2.79
3,3'-dichlorobenzidine	3.92E-04	Hansler and Posthumus, in prep.	EqP	41.17	2.85

[a]An *ad hoc*-MPC for pentaBDE was not derived by RIVM since finalisation of the EU-RAR for this substance (group) was anticipated.
[b]No *ad hoc*-MPCs derived by RIVM since a TV (target value) for DNOC already existed.

5.5 *Ad hoc*-MPCs for sediment

Ad hoc-MPC values for sediment have been derived only by RIVM, not by RIZA. The *ad hoc*-MPC values for sediment are equal to the *ad hoc*-MPC values for soil and are presented in Table 55.

6. Toxicity data and ERL derivation for water

6.1 ERL derivation for water

6.1.1 PentaBDE

Since this ERL derivation is based on the WFD data sheet and the EU-RAR (where appropriate), some terminology from both frameworks may be found in the following ERL derivation of pentaBDE; e.g. PNEC (predicted no effect concentration) and QS (quality standard).

6.1.1.1 $MPC_{eco, water}$

This section is cited from the WFD fact sheet (Anonymus, 2005a), which is identical to the derivation reported in EC (2001). Aquatic toxicity data for pentaBDE are tabulated in Table A5. 1 (acute, freshwater) and Table A5. 19 (chronic, freshwater) in Appendix 5. Data selected for ERL derivation are tabulated in Table A1. 1 in Appendix 1.

Freshwater

Long-term NOECs are available for three aquatic species, representing three trophic levels. Therefore, an assessment factor of 10 is applied to the lowest of the available NOECs. The lowest NOEC is 5.3 $\mu g.L^{-1}$ for *Daphnia magna* (Drottar and Krueger (1998), in Anonymus, 2004). This results in a $PNEC_{aqua} = MPC_{eco, water}$ of 5.3 $\mu g.L^{-1}$ / 10 = 0.53 $\mu g.L^{-1}$.

Marine

Since no data on specific marine taxa are available, an assessment factor of 100 is applied to the lowest NOEC, resulting in an $MPC_{eco, marine}$ of 0.053 $\mu g.L^{-1}$.

6.1.1.2 $MPC_{sp, water}$

This section deviates from the derivation of the AA-QS from Anonymus (2004) and the PNEC derivation reported in EC (2001), since human toxicological risk limit derived by De Winter-Sorkina *et al*. (2006) was used (see section 4.1.3).

Freshwater

In the EU-RAR, EUSES calculations were carried out using the BCF from the original study (14350 $L.kg^{-1}$), but the recalculated value of 27400 $L.kg^{-1}$ was also taken into consideration in the risk assessment. The latter value was therefore used for ERL derivation. A BMF_1 of 20 is selected as highest value of a range, determined in a fish reproduction study.
An assessment factor of 3 was applied to convert the LOAEL of 60 $\mu g.kg_{bw}^{-1}.d^{-1}$ to a NOAEL of 20 $\mu g.kg_{bw}^{-1}.d^{-1}$. A conversion factor for food intake of 20 $g_{bw}.g_{fd}^{-1}.d^{-1}$ and an assessment factor of 30 (both factors taken from INS and TGD guidance) are applied to reach an $MPC_{oral, min}$ of 13.3 $\mu g.kg_{fd}^{-1}$. Using this $MPC_{oral, min}$ and the abovementioned data, results in an $MPC_{sp, water}$ of 24.3 $pg.L^{-1}$.

Marine

Following the same derivation as for freshwater, using the extra BMF_2 of 10, results in an $MPC_{marine, sp}$ = 2.43 $pg.L^{-1}$.

6.1.1.3 $MPC_{hh\ food,\ water}$

The human toxicological risk limit derived by De Winter-Sorkina *et al*. (2006) is used (see section 4.1.3). Using the equations and defaults from INS guidance and the TL_{hh} of 0.26 $ng.kg_{bw}^{-1}.d^{-1}$ based on reproductive effects resulted in an $MPC_{hh\ food}$ of 15.8 $ng.kg_{fd}^{-1}$. Using this $MPC_{hh\ food}$, BCF = 27400 $L.kg^{-1}$ and BMF_1 = 20, the resulting $MPC_{hh\ food,\ water}$ is 0.029 $pg.L^{-1}$.

6.1.1.4 $MPC_{dw,\ water}$

A provisional drinking-water standard is calculated on basis of TGD methodology, using the TL_{hh} of 0.26 $ng.kg_{bw}^{-1}.d^{-1}$. The $MPC_{dw,\ water,\ provisional}$ = (0.1*0.26*70/2=) 0.91 $ng.L^{-1}$

The WFD datasheet of pentaBDE (Anonymus, 2004) states that the provisional drinking-water quality standard is by far higher than the standard required to protect human health from adverse effects by food uptake or the aquatic community. For this reason, it was decided not necessary to derive a quality standard for drinking-water abstraction.

6.1.1.5 Selection of the MPC_{water}

Freshwater

The following MPC_{water} were derived for pentaBDE:
$MPC_{eco,\ water}$ = 530 $ng.L^{-1}$
$MPC_{sp,\ water}$ = 0.024 $ng.L^{-1}$
$MPC_{hh\ food,\ water}$ = 0.000029 $ng.L^{-1}$ (0.029 $pg.L^{-1}$)
$MPC_{dw,\ water}$ = 0.91 $ng.L^{-1}$

The $MPC_{hh\ food,\ water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for pentaBDE is 0.029 $pg.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine

For the marine environment the following MPCs were determined:
$MPC_{eco,\ marine}$ = 53 $ng.L^{-1}$
$MPC_{marine,\ sp}$ = 0.0024 $ng.L^{-1}$
$MPC_{hh\ food,\ water}$ = 0.000029 $ng.L^{-1}$ (0.029 $pg.L^{-1}$)

The lowest value is selected as MPC_{marine}: 0.029 $pg.L^{-1}$. This value reflects the total concentration (see section 1.4.1).

6.1.1.6 MAC_{eco}

In the datasheet for pentaBDE, the MAC-QS is based on the lowest acute toxicity value of 14 $\mu g.L^{-1}$ for *Daphnia magna*. A reduced AF of 10 is applied, instead of an AF of 100. The resulting MAC-QS is 1.4 $\mu g.L^{-1}$. The reduction of the AF is based on available NOECs for algae, which are 'in the worst case two times higher than the proposed MAC-QS'.

In our opinion, this MAC value is questionable, with respect to the guidance given (Lepper, 2005; EC-JRC, 2003). For compounds having the potential to bioaccumulate, which is the case for pentaBDE, an assessment factor of 100 'may not always be sufficient to provide adequate protection'. Moreover, for the derivation of the MAC_{eco}-value, at least one short-term L(E)C50 value from each of the three trophic levels of the base-set should be available. This is not the case for pentaBDE. We conclude that derivation of an MAC_{eco} for pentaBDE is not possible.

6.1.1.7 SRC_{eco}

Freshwater

Since chronic toxicity data are available for three trophic levels, the $SRC_{eco, water}$ is calculated as the geometric mean of chronic data (see Table A1. 1 in Appendix 1). The resulting $SRC_{eco, water} = 0.0060$ mg.L^{-1} or 6.0 µg.L^{-1}.

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine} = 6.0$ µg.L^{-1}.

6.1.2 p-*tert*-Octylphenol

6.1.2.1 $MPC_{eco, water}$

The extensive assessment of studies on endocrine mediated responses of p-*tert*-octylphenol as given in Brooke *et al*. (2005) (and summarised in the WFD fact sheet) will not be repeated here. We refer to the report of Brooke *et al*. and the WFD fact sheet (Anonymus, 2005a) for detailed information.

The ERL derivation presented here is cited from Anonymus (2005a), which is based on the data presented in Brooke *et al*. Aquatic toxicity data for OP are tabulated in Table A5. 2 (acute, freshwater) and Table A5. 13 (acute, marine), while chronic data are presented in Table A5. 20. (freshwater). Data selected for ERL derivation are tabulated in Table A1. 2.

Freshwater

The base set is complete and chronic toxicity data are available for the three trophic levels of the base set. However, the available data for algae are considered to be 'use with care data' by Brooke *et al*. The lowest NOEC (growth) is 6.1 µg.L^{-1}, found for the rainbow trout *Oncorhynchus mykiss*. An acute toxicity test result (EC50, immobilisation) of 13.3 µg.L^{-1} is available for *Gammarus pulex*. Because this is the lowest acute toxicity test result and a chronic study is not available for this species an assessment factor of 50 has been applied to the lowest NOEC to derive the $PNEC_{aqua}$. An extra argument put forward to underpin this assessment factor is the observation that algae and invertebrates are more sensitive to nonylphenol than fish.

We do not fully agree with the above reasoning (comments outlined in a separate section on p. 82). However, we have decided not to deviate from the ERL derivation presented in the WFD fact sheet (and Brooke *et al*.) since we have not performed an evaluation of data for p-*tert*-octylphenol. The PNEC will be used as MPC: $MPC_{eco, water}$ is 6.1/50 = 0.122 µg.L^{-1}.

Consideration of data on endocrine disruption

The lowest valid NOEC for an endocrine mediated response is 12 µg.L^{-1} for several endpoints relating to reproductive success (time to first spawning, total number of eggs per female and per day, fertilisation capacity and cumulative number of fertilised eggs) from a life cycle study with *D. rerio*. This NOEC is higher than the lowest NOEC for *O. mykiss* which is used to derive the MPC. It is concluded that on the basis of valid studies, the $MPC_{eco, water}$ is protective for endocrine mediated effects at the population level.

Effect concentrations at lower concentrations have been established in less valid (as judged by Brooke *et al*.) studies focusing on parameters not directly related to the population level. The lowest NOEC for effects on VTG production in fish was 1.6 µg.L^{-1}. Data from less valid studies gave the following effect levels: a possible NOEC of 1 µg.L^{-1} (increase in embryo production) for the freshwater mollusc (snail) *Potamopyrgus antipodarum*; a LOEC (lowest observed effect

concentration) of 0.01 µg.L^{-1} (endpoint: delay in completion of naupliar stage in F_1 generation) of the estuarine copepod *Tigriopus japonicus*; and a LOEC of 0.2 µg.L^{-1} (endpoint: developmental changes) of the bullfrog *Rana catesbeiana*. Combining the lesser validity of the studies summarised and the observation that the $MPC_{eco, water}$ is lower than most of the effect concentrations mentioned, the height of the MPC was considered to be valid.

INS - Considerations against the use of an assessment factor of 50
If one considers the 'use with care' algal toxicity studies as valid for ERL derivation, the base set is complete, and NOECs are available at the three trophic levels represented by the base set. An assessment factor of ten may then be applied to the lowest toxicity test result.
Brooke *et al*. argue that an assessment factor of 50 should be applied to the NOEC found for fish (*O. mykiss*), following the reasoning that the LC50 for *G. pulex* was the lowest acute toxicity test result and a chronic test is not available for this species. However, the TGD states that an assessment factor may be applied to the lowest NOEC in such a case, only when the lowest LC50 is generated from a trophic level which is not represented in the chronic toxicity data. This is not the case. *Gammarus pulex* is a crustacean, an invertebrate species belonging to the trophic level of primary consumers. A chronic toxicity study is available for this trophic level (*Daphnia magna*). The fact that the acutely most sensitive *species* belonging to one of the three demanded trophic levels in the base set is not represented in the three trophic levels of the chronic data is not a reason to increase the assessment factor.

Brooke *et al*. have also used a more conservative assessment factor than the TGD prescribes because of the potential higher sensitivity of algae and invertebrates to octylphenol in chronic tests. This higher sensitivity does not show from the algal toxicity data tabulated for octylphenol. Although a 'use with care' value, the EC10 value for *Scenedesmus subspicatus* of 300 µg.L^{-1} is a factor of 5 higher than the NOEC for *D. magna* and a factor of 50 higher than the NOEC for *O. mykiss*. The NOEC from the chronic invertebrate (*Daphnia*) study is a factor of 10 higher than the NOEC from the fish study.
Moreover, it should be noted that the presumed accordance with the sensitivity pattern for nonylphenol is feeble. The PNEC for nonylphenol from the EU-RAR (EC, 2002) was indeed based on an algal study (EC10 of 3.3 µg.L^{-1}). Note that the EU-RAR for nonylphenol dates from 2002. A recent study by Lahnsteiner *et al*. (2005) reports a NOEC of 0.13 µg.L^{-1} for fish (*O. mykiss*), showing that algae are not necessarily one of the most sensitive taxa.

On the other hand, the data on endocrine mediated effects from less relevant and/or less valid studies (see section *Consideration of data on endocrine disruption*) very clearly indicates the possibility of effects occurring at much lower concentrations than the NOEC of 6.1 µg.L^{-1} found for *O. mykiss*. This information might be used to lower the applied assessment factor. However, this information was not explicitly used in the argumentation to increase the assessment factor from 10 to 50. We consider these presence of the results on endocrine mediated effects sufficient argumentation to agree with the policy of a higher assessment factor.

Marine
Only acute saltwater toxicity data are available for p-*tert*-octylphenol. Brooke *et al*. consider the available dataset on toxicity of octylphenol to marine organisms insufficient to allow for a different interpretation to that for freshwater. No data from additional marine taxonomic groups are available. The $MPC_{eco, marine}$ is based on the same dataset as the MPC freshwater. The resulting $MPC_{eco, marine}$ is 6.1 / 100 = 0.061 µg.L^{-1}.

Brooke *et al*. use an assessment factor of 500 for the derivation of the $PNEC_{marine}$ following the same reasoning as described in the section on MPC freshwater derivation. NOEC values from 1 to 11.5 $\mu g.L^{-1}$ from tests aimed at endocrine disrupting effects are cited to emphasise an apparent higher sensitivity. However, these endpoints of these NOECs are not representative at the population level. This is an important criterion that is used within INS framework for selection of test results.

6.1.2.2 $MPC_{sp, water}$

Freshwater

Data used for derivation of and ERL for secondary poisoning are cited from Brooke *et al*. (2005). From the NOAEL of 15 $mg.kg_{bw}^{-1}.d^{-1}$ (see section 4.2.34.3.3), an $MPC_{oral, min}$ of 10 $mg.kg_{fd}^{-1}$ is derived using a conversion factor of 20 (rats > 6 weeks of age) and an assessment factor of 30 (chronic mammal study). Using this $MPC_{oral, min}$, a BCF of 634 $L.kg^{-1}$ (section 4.2.1), and a BMF_1 of 1, the $MPC_{sp, water}$ is calculated to be 15.8 $\mu g.L^{-1}$.

Marine

Since the BMF_2 is also 1, the marine $MPC_{sp, water}$ is equal to the $MPC_{sp, water}$ for freshwater.

6.1.2.3 $MPC_{hh\ food, water}$

The OECD SIDS (OECD, 1995) document is the only source that could be retrieved which has published a human health related toxicological standard. An ADI of 0.05 $mg.kg_{bw}^{-1}.d^{-1}$ is reported, based on a NOAEL of 15 $mg.kg_{bw}^{-1}.d^{-1}$ (liver effects in a 28 day repeated dose OECD 407 study) and an assessment factor of 300. The value of the NOAEL used in the OECD report is equal to the value of the NOAEL reported by Brooke *et al*., although the NOAEL derived in the latter report is based on more and more valid studies.

The WFD fact sheet does not mention the ADI from the OECD-SIDS document. Since it was decided to use the ERLs as derived in the WFD fact sheet, a TL_{hh} of 0.15 $mg.kg_{bw}^{-1}.d^{-1}$ is used, derived by applying the standard assessment factor of 100 is to the NOAEL of 15 $mg.kg_{bw}^{-1}.d^{-1}$. Using the TL_{hh} of 0.15 $mg.kg_{bw}^{-1}.d^{-1}$, an $MPC_{hh, food}$ of 9.13 $mg.kg_{fd}^{-1}$ is derived. Using the BCF of 634 $L.kg^{-1}$ and $BMF_1 = 1$, the resulting $MPC_{hh\ food, water}$ **= 14.40 $\mu g.L^{-1}$**.

NB. The WFD fact sheet follows the same calculation, but has rounded off halfway the calculation ($0.15 \times 70 = 1.05$ was rounded to 1), thus resulting in a lower $QS_{water, hh\ food}$ of 13.7 $\mu g.L^{-1}$.

6.1.2.4 $MPC_{dw, water}$

Using the TL_{hh} of 0.15 $mg.kg_{bw}^{-1}.d^{-1}$, an $MPC_{dw, water}$ of 0.525 mgL^{-1} (525 $\mu g.L^{-1}$) is derived.

6.1.2.5 Selection of the MPC_{water}

Freshwater

The following MPC_{water} were derived for p-*tert*-octylphenol:

$MPC_{eco, water} = 0.122\ \mu g.L^{-1}$

$MPC_{sp, water} = 15.8\ \mu g.L^{-1}$

$MPC_{hh\ food, water} = 14.4\ \mu g.L^{-1}$

$MPC_{dw, water} = 525\ \mu g.L^{-1}$

The $MPC_{eco, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for p-*tert*-octylphenol is 0.12 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine

For the marine environment the following MPCs were determined:

$MPC_{eco, marine}$ = 0.012 µg.L^{-1}
$MPC_{marine, sp}$ = 16 µg.L^{-1}
$MPC_{hh\ food, water}$ = 14.4 µg.L^{-1}

The lowest value is selected as MPC_{marine}: 0.012 µg.L^{-1} or 12 ng.L^{-1}. This value reflects the total concentration (see section 1.4.1).

6.1.2.6 MAC_{eco}

The MAC_{eco} is cited from the WFD fact sheet on p-*tert*-octylphenol (Anonymus, 2005a). The lowest acute toxicity test result is an EC50 of 13.3 µg.L^{-1} for immobilisation of *Gammarus pulex*. An assessment factor of 100 is applied to derive the MAC_{eco}. Therefore, MAC_{eco} = 0.133 µg.L^{-1}.

6.1.2.7 SRC_{eco}

Freshwater

The toxicity data presented in Brooke *et al*. are tabulated in Table A5. 2 and Table A5. 13. A single value per species was derived, as presented in Table A1. 2. Since NOECs are available for more than three taxa, the SRC_{eco} for the aquatic compartment is calculated as the geometric mean of the chronic toxicity data. SRC_{eco} = 0.0408 mg.L^{-1} = 40.8 µg.L^{-1}.

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine}$ = 40.8 µg.L^{-1}.

6.1.3 Benzo[*b*]fluoranthene

The MPC derivation reported in section 6.1.3.1 is based on the draft EU-RAR for coal tar pitch (EC, 2006b).

6.1.3.1 $MPC_{eco, water}$

Aquatic toxicity data for benzo[*b*]fluoranthene are tabulated in Table A5. 3 (acute, freshwater) and Table A5. 21 (chronic, freshwater). Data selected for ERL derivation are tabulated in Table A1. 3 in Appendix 1. No data on marine species are available.

Freshwater

Citation from draft EU-RAR on PCTHT (EC, 2006b):
'Some acute toxicity studies for benzo[*b*]fluoranthene have been performed with *Daphnia magna*. In a standard 48-h study performed in the dark, no toxicity was found up to 1.1 µg.L^{-1} (Bisson *et al*., 2000). In a 24-h study with a photoperiod 16:8 hour light: dark no toxicity was found either. In the same treatment but extended with 2 hours of irradiation with UV light (295-365 nm; peak 340 nm) with an intensity of 370 ± 20 µW.cm^{-2} and a recovery period of 2 hours, the EC50 for immobility was 4.2 µg.L^{-1} (Wernersson & Dave, 1997). This is still above the aqueous solubility of 1.1-1.5 µg.L^{-1} (Mackay *et al*., 2000). No toxic effects were observed as well in two chronic toxicity studies with the alga *Pseudokirchneriella subcapitata* and the crustacean *Ceriodaphnia dubia* (Bisson *et al*., 2000).'

The draft EU-RAR concludes that the only value that can be used to derive the PNEC is the LC50 for *Daphnia magna*, which is above the aqueous solubility. For this reason, it was proposed to use the same PNEC for benzo[*b*]fluoranthene as for benzo[*k*]fluoranthene.

Toxicity data for benzo[k]fluoranthene
Aquatic toxicity data for benzo[*k*]fluoranthene are tabulated in Table A5. 4 (acute, freshwater) and Table A5. 22 (chronic, freshwater). Data selected for ERL derivation are tabulated in Table A1. 4 in Appendix 1. No data on marine species are available.
Citation from draft EU-RAR on PCTHT (EC, 2006b):
'Acute toxicity data for benzo[*k*]fluoranthene are only available for *Daphnia magna*. In the two available studies (Bisson *et al*., 2000; Verrhiest *et al*., 2001) no effects were observed. However, due to the low solubility of benzo[*k*]fluoranthene of about 1 $\mu g.L^{-1}$ (Mackay *et al*., 2000), acute effects are not anticipated. For algae no EC50 is presented. However, in the 72-h study with *Pseudokirchneriella subcapitata*, the EC10 for growth is higher than 1 $\mu g.L^{-1}$ (Bisson *et al*., 2000), hence the EC50 must also be higher than this value. In the 7-d reproduction study with *Ceriodaphnia dubia*, no effects were observed either (Bisson *et al*., 2000). In two studies, the effects of benzo[*k*]fluoranthene in an ELS test with *Brachydanio rerio* was examined. In the first 28-d study one concentration of 0.58 $\mu g.L^{-1}$ was tested. At this concentration, 52% mortality occurred (Hooftman & Evers-de Ruiter, 1992b). In a second 42-d study, a dose-response relationship was examined. The mentioned concentrations here are based on measured concentrations per concentration and not on average recovery times the nominal concentration, as given in the report. The LC50 estimated from the presented data with a log-logistic relationship was 0.65 $\mu g.L^{-1}$. From the data for weight and length EC10 values are derived of 0.31 and 0.17 $\mu g.L^{-1}$. Due to the good fit of the log-logistic equation, these estimates have a low uncertainty.'

'Although the base-set is not complete, because acute toxicity data for fish are missing, an assessment factor of 10 is considered suitable, because chronic toxicity data are available for algae, crustaceans and fish. The most sensitive endpoint is length of *Brachydanio rerio* in an ELS test. The EC10 for this endpoint is 0.17 $\mu g.L^{-1}$. With an assessment factor of 10, the PNEC for freshwater is 0.017 $\mu g.L^{-1}$'.

Marine
The $MPC_{eco,\ marine}$ is taken over from the $PNEC_{marine}$ as derived in the RAR.
$MPC_{eco,\ marine}$ = 0.0017 $\mu g.L^{-1}$ or 1.7 ($ng.L^{-1}$).

Citation from draft EU-RAR on PCTHT (EC, 2006b):
'Evaluation of the applied assessment factors
For the majority of the PAHs sufficient toxicity data are available in order to apply an assessment factor of 10 on the most sensitive endpoint found for that particular PAH. For pyrene, benzo[*a*]anthracene, benzo[*b*]fluoranthene, dibenzo[*a,h*]anthracene and indeno[1,2,3-*cd*]pyrene less toxicity data are available and consequently higher assessment factors are applied following the general recommendation of the EU TGD. In the section below the possibility of applying lower assessment factors are investigated, by read-across with data available for the other PAHs.

Benzo[*b*]fluoranthene
An assessment factor of 1000 to the lowest acute EC_{50} has been used for benzo[*b*]fluoranthene, because the base-set is not complete for this compound. Two chronic NOECs for two trophic levels are available. These are the EC_{10} for growth of the algae *Pseudokirchneriella subcapitata* and for reproduction of the crustacean *Ceriodaphnia dubia* (Bisson *et al*., 2000). However, no EC_{10} could be established in these studies. On the other hand, it appeared that benzo[*b*]fluoranthene is phototoxic to *Daphnia magna* (Wernersson & Dave, 1997). In other cases where enough data are available but still phototoxicity appears to be the most sensitive endpoint an assessment factor of 10 has been applied to the lowest EC_{50} (e.g. for anthracene and fluoranthene). However, in several

cases the EC_{50} for phototoxicity to *Daphnia magna* (Wernersson & Dave, 1997) appears to be more than a factor of 10 higher than the lowest endpoint for those compounds, e.g. for fluoranthene a factor of 350, for B[*a*]P a factor of 39, for dibenzo[*a,h*]anthracene a factor of 33, and for pyrene a factor of 25. In this case, a comparison can better be made with its isomer benzo[*k*]fluoranthene. A toxicity test with *Daphnia magna* showed that this compound is also not very phototoxic, because no effects were observed up to the limit of solubility after irradiation with UV-A radiation (Verrhiest *et al*., 2001). For benzo[*k*]fluoranthene, toxicity tests are available for algae, Daphnids and fish. The lowest result was found for fish, the trophic level for which no data are available for benzo[*b*]fluoranthene. Benzo[*k*]fluoranthene and benzo[*b*]fluoranthene are mostly reported together. Therefore, it was proposed to use the same PNEC for benzo[*b*]fluoranthene as for benzo[*k*]fluoranthene.'

6.1.3.2 $MPC_{sp, water}$

Freshwater and marine

Since an MPC_{oral} for birds and/or mammals has not been derived in the draft EU-RAR (see section 4.3.3.2), secondary poisoning for benzo[*b*]fluoranthene can not be assessed.

6.1.3.3 $MPC_{hh\ food, water}$

Freshwater

Since a BCF for benzo[*b*]fluoranthene has not yet been derived in the draft EU-RAR, an $MPC_{hh\ food, water}$ can not be derived.

6.1.3.4 $MPC_{dw, water}$

Since an A1 value is available from 75/440/EC (EC, 1975), this value determines the $MPC_{dw, water}$. However, the listed A1 value is 0.2 $\mu g.L^{-1}$ (200 $ng.L^{-1}$) for 'Polycyclic aromatic hydrocarbons'. This is rather undefined, since (i) it is not clarified which individual PAHs are considered to belong to the group of 'Polycyclic aromatic hydrocarbons', and (ii) the A1 value stands for the summed concentrations of PAHs present in surface water. However, a sum-standard can not be used to derive a standard for an individual compound.

If an A1 value for a compound is not available, FHI guidance prompts to use a DW standard from CD 98/83/EC (EC, 1998). However, the DW standard of 0.1 $\mu g.L^{-1}$ is also a sum standard, for four PAHs (benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]fluoranthene and indeno(1,2,3-cd)pyrene).
Since both the A1 value and the DW standard can not be used to set an $MPC_{dw, water}$ for a single PAH, we have therefore derived an $MPC_{dw, water, provisional}$ according to FHI guidance. Using the human toxicological threshold limit (TL_{hh}) of 50 $ng.kg_{bw}^{-1}.d^{-1}$ (section 4.3.4), the $MPC_{dw, water, provisional}$ is calculated to be 175 $ng.L^{-1}$.

6.1.3.5 Selection of the MPC_{water}

Freshwater

The following MPC_{water} were derived for benzo[*b*]fluoranthene:
$MPC_{eco, water}$ = 17 $ng.L^{-1}$
$MPC_{dw, water, provisional}$ = 175 $ng.L^{-1}$

Note

The $MPC_{eco, water}$ is the lowest value of the available MPC_{water} values. Therefore, the MPC_{water} is 17 $ng.L^{-1}$. However, since the EU-RAR on coal tar pitch (EC, 2006b) is still in draft at the time of

reporting, it is strongly advised to treat the MPC_{water} as preliminary. After finalisation of the EU-RAR, a final MPC_{water} can be derived.
Since the $MPC_{eco, water}$ is 17 $ng.L^{-1}$ and the human toxicological threshold limit is known (TL_{hh} = 50 $ng.kg_{bw}^{-1}.d^{-1}$) and BMF is set at 1 (section 4.3.3.1), it can be derived what value for the BCF is needed to derive an $MPC_{hh\ food, water}$ that is lower than the $MPC_{eco, water}$. Using the FHI equations for $MPC_{hh\ food, water}$, a BCF of at least 179 $L.kg^{-1}$ is calculated. This means that a BCF of at least 179 $L.kg^{-1}$ is needed to derive an MPC_{water} that is lower than the one currently proposed on the basis of ecotoxicological data. Since the consumption of mussels should also be covered by this route, and the fact that mussels have low biotransformation capacity for PAHs (and thus higher BCF values are expected) a lower MPC_{water} for benzo[*b*]fluoranthene is to be expected.

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco, marine}$ = 1.7 $ng.L^{-1}$

The $MPC_{eco, water}$ is the lowest value of the available MPC_{water} values. Therefore, the MPC_{water} is 17 $ng.L^{-1}$. However, since the EU-RAR on coal tar pitch (EC, 2006b) is still in draft at the time of reporting, it is strongly advised to treat the MPC_{water} as indicative. After finalisation of the EU-RAR, a final MPC_{water} can be derived.

6.1.3.6 MAC_{eco}
Prerequisite for MAC_{eco} derivation is, that test results from at least 3 short term tests for three tropic levels ('base set') are available. As with the MPC derivation, toxicity data for both benzo[*k*]fluoranthene and benzo[*k*]fluoranthene have been taken into consideration. However, the base set is not complete, therefore a MAC_{eco} can not be derived for benzo[*b*]fluoranthene.

6.1.3.7 SRC_{eco}
Freshwater
As with the derivation of the MPC, toxicity data for both benzo[*b*]fluoranthene and benzo[*k*]fluoranthene were used to derive the SRC_{eco}. One acute toxicity study resulting in a useful endpoint is available, i.e. an EC50 of 4.2 $\mu g.L^{-1}$ for *D. magna*. In addition, one chronic toxicity study resulting in a useful endpoint is available, i.e. an EC10 of 0.17 $\mu g.L^{-1}$ for *B. rerio*. The toxicity result from the chronic study is lower than the acute result divided by an assessment factor of 10: 0.17 $\mu g.L^{-1}$ vs. 0.42 $\mu g.L^{-1}$, respectively. The lowest value is selected, therefore the SRC_{eco} is 0.17 $\mu g.L^{-1}$.

Marine
The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine}$ = 0.17 $\mu g.L^{-1}$.

6.1.4 Isodrin
Freshwater
The Σ MPC_{water} for the four drins (aldrin, dieldrin, endrin and isodrin) is 10 $ng.L^{-1}$. This environmental quality standard for water was set in 88/347/EEC (EC, 1988), a daughter Directive of 76/464/EEC (EC, 1976). This standard is still in force under 2000/60/EC (EC, 2000) and its draft daughter Directive COM (2006) 397 (EC, 2006a). See also section 3.1.4.

Marine
The Σ MPC_{marine} for the four drins (aldrin, dieldrin, endrin and isodrin) is 5 $ng.L^{-1}$. This environmental quality standard for marine water was set in 88/347/EEC (EC, 1988), a daughter Directive of 76/464/EEC (EC, 1976). This standard is still in force under 2000/60/EC (EC, 2000) and its draft daughter Directive COM (2006) 397 (EC, 2006a). See also section 3.1.4.

The sum standard for the group of four drins means that concentration measurements for isodrin should always be accompanied with measurements of dieldrin, aldrin and endrin. The MPC_{water} for isodrin is maximally 10 $ng.L^{-1}$, in case only isodrin is measured and dieldrin, aldrin and endrin are not detected. In case any of the other drins is present in water samples, the total concentration should not exceed 10 $ng.L^{-1}$.

6.1.5 DNOC

6.1.5.1 $MPC_{eco, water}$

Aquatic toxicity data for DNOC can be found in Table A5. 5 (acute, freshwater), Table A5. 14 (acute, marine), Table A5. 23 (chronic, freshwater) and Table A5. 31 (chronic, marine) in Appendix 5. Data used for ERL derivation are reported in table Table A1. 5 in Appendix 1. WFD guidance, published by the Fraunhofer Institute and implemented in INS guidance (Van Vlaardingen and Verbruggen, 2007) states that for ERL derivation for plant protections products, freshwater and marine toxicity data should not be pooled. Therefore, toxicity data for marine species are not considered for freshwater ERLs derivation and *vice versa*.

Freshwater
The base set is complete and the set of chronic toxicity data fulfils the criteria for refined effect assessment: data for bacteria, cyanobacteria, algae, protozoa, macrophyta, coelenterata, rotifera, mollusca, crustacea, insecta, pisces and amphibia are present. The MPC is derived using refined effect assessment.

A lognormal species sensitivity distribution (SSD) was fitted through the chronic toxicity data according to the method of Aldenberg and Jaworska (Aldenberg and Jaworska, 2000), using the software program *ETX* 2.0 (Van Vlaardingen *et al.*, 2004). The SSD is presented in Figure 14. The sample of 23 toxicity test results passes all three tests on (log)normal distribution, indicating that the application of the extrapolation method is justified. A median HC_5 of 28 $\mu g.L^{-1}$ (90% confidence interval: 5.2 – 89 $\mu g.L^{-1}$) is calculated for this DNOC.

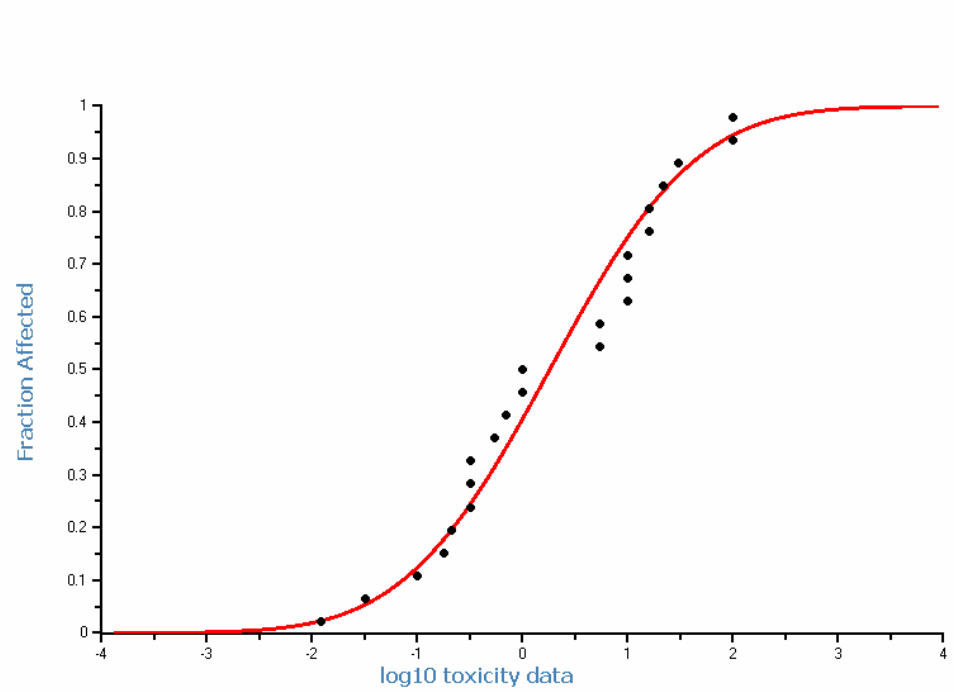

Figure 14. Species sensitivity distribution of chronic DNOC toxicity to aquatic freshwater organisms. HC_5 = 28 µg.L^{-1} (90% CI: 5.2-89); n=23.

Application of an assessment factor to the HC_5

- *Data quality.* All toxicity data have been retrieved from peer reviewed scientific journal and are therefore be considered of good quality. However, the majority of test results is based on nominal concentrations. This has two disadvantages: (i) there is no verification whether or not the intended concentration was actually achieved in the test (experimental errors are not detected) and (ii) there is no indication on how the concentration changes during the exposure period. With respect to the first point, it can be argued that values based on nominal concentrations are not less reliable *per se*. The lack of the possibility to detect errors should be noted, but this is a reason to treat studies differently. (N.B. this also depends on the properties of the compound under investigation.) Moreover, the higher the amount of studies used, the smaller the chance that in multiple studies experimental errors have been committed. In the case of DNOC, studies with longer duration for several taxonomic groups (coelenterata, mollusca, crustacea, insecta, pisces, amphibia) were renewal studies, which makes errors in concentrations less likely.
  With respect to the point of concentration change, the relevance of this item depends on the compound properties, the duration of the exposure and the type of exposure (static, renewal, flow-through). In the case of DNOC, all longer exposures were either renewal (majority) or continuous flow. Furthermore, sorption to glassware is not expected to be high for DNOC because of the fact that it occurs in the ionised form at pH values around 7 and its log K_{ow} is relatively low (2.13). Taking the above information together, it is concluded that data quality is not optimal because of nominal concentrations, but this is thought to have a minor influence on the reliability of the HC_5. A small increase of the assessment factor is proposed to cover this uncertainty.
- *Diversity of taxa in SSD.* Organisms of various trophic levels are represented in the data set, which is therefore considered to be an adequate reflection of the aquatic ecosystem.

- *Mode of action*. The mode of action of DNOC is uncoupling of oxidative phosphorylation. Oxidative phosphorylation is the process in which energy contained in organic molecules is released by their stepwise –biochemical– oxidation and ultimately transformed into ATP (adenosine triphosphate). This process is carried out by prokaryotic as well as eukaryotic species. In that respect, DNOC is potentially toxic to a very large group of organisms.
- *Statistical uncertainty in HC_5*. The statistical uncertainty in the HC_5 is expressed in e.g. its 90% confidence interval, which ranges from 4 to 68 $\mu g.L^{-1}$, which the median estimate HC_5 being 28 $\mu g.L^{-1}$. The SSD fits well to the experimental data, since three goodness-of-fit tests were passed at all levels of significance.
- *Mesocosm/field studies*. No mesocosm or field studies were retrieved for DNOC.
- *NOEC values below the HC_5.* One NOEC value is lower than the HC_5, which is the NOEC of 12 $\mu g.L^{-1}$ for the protozoan *Uronema parduczi*. This value is based on a static test (no renewal), on nominal test concentrations and exposure lasted 20 hours.

Taking into account that several nominal values are included in the dataset and that there is one NOEC below the HC_5, we consider the application of an assessment factor of 3 valid. The MPC for DNOC is therefore equal to 27.5/3 = 9.2 $\mu g.L^{-1}$ (the non rounded off value of the HC_5 is used).

Newman *et al*., (2000) have also derived an HC_5 value for DNOC using chronic toxicity data (NOEC values, n=21), assuming a lognormal distribution of the data. The distribution of their data corresponded to a lognormal distribution (Shapiro-Wilk's test, p=0.06) and an HC_5 value of 44 $\mu g.L^{-1}$ was calculated. The underlying dataset was not presented, although the data of Slooff and Canton (1983) were included in their SSD as is the case in the SSD we present here. The difference between the HC_5 calculated by Newman and the HC_5 derived here is less than a factor of two, which is considered acceptable.
Okkerman *et al*. (1991) reported an HC_5 of 10 $\mu g.L^{-1}$ using a different extrapolation technique (method of Van Straalen and Denneman) and chronic toxicity data for DNOC (n=11) published by Slooff and Canton (1983). The HC_5 of this dataset determined using the method of Aldenberg and Jaworska is 33 $\mu g.L^{-1}$. The toxicity data by Slooff and Canton have also been used in the ERL derivation presented here, but some of these data were averaged with other results for identical species, and more NOECs were added to the total data set. This has resulted in a somewhat lower HC_5 of 28 $\mu g.L^{-1}$.

Marine
Acute toxicity data are available for bacteria and fish. One chronic toxicity test result for a marine species was available (*Vibrio fischeri*). This is a very marginal data set. To allow for ERL_{marine} derivation, it should be established 'with high probability' (FHI guidance) that marine organisms are not more sensitive than freshwater organisms. In this case, acute toxicity data for freshwater bacteria are not available for comparison with marine data. Furthermore, there is only one acute marine fish test result and only one chronic marine test result. Single data can not be used to conclude 'with high probability' on differences in sensitivity.
In this case, FHI guidance concludes that an ERLs for the marine compartment can not be derived. Thus, an MPC_{marine} for DNOC is not derived here.

6.1.5.2 $MPC_{sp, water}$
DNOC has no potential for bioaccumulation: an $MPC_{sp, water}$ is not derived (section 4.5.2).

6.1.5.3 $MPC_{hh\ food, water}$
DNOC has a log K_{ow} < 3 and no relevant R classification: an $MPC_{hh\ food, water}$ is not derived (section 4.5.2).

6.1.5.4 $MPC_{dw, water}$

An A1 value of 1 $\mu g.L^{-1}$ for the sum of 'total pesticides' is set (section 4.5.2). However, this A1 value stands for 'Total pesticides'. Since it is not possible to derive a standard for an individual compound from this group we propose to use the DWS for pesticides from CD 98/83/EC (EC, 1998), which is 0.1 $\mu g.L^{-1}$.

6.1.5.5 Selection of the MPC_{water}

Freshwater

The following MPC_{water} were derived for DNOC:
$MPC_{eco, water}$ = 9.2 $\mu g.L^{-1}$
$MPC_{dw, water}$ = 0.1 $\mu g.L^{-1}$

The $MPC_{dw, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for DNOC is 0.1 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine

For the marine environment no MPC is derived.

6.1.5.6 MAC_{eco}

DNOC has no bioaccumulation potential. The mode of action of DNOC is known, however, interspecies variation is not considered to be low since the range of acute toxicity test results spans over three orders of magnitude. An assessment factor of 100 is applied to the lowest acute test result (LC50 of 0.066 $mg.L^{-1}$ for *O. mykiss*) to derive the MAC_{eco}. MAC_{eco} = 66/100 = 0.66 $\mu g.L^{-1}$.

6.1.5.7 SRC_{eco}

Freshwater

Since NOECs are available for more than three taxa, the SRC_{eco} for the aquatic compartment is calculated as the geometric mean of the chronic toxicity data. SRC_{eco} = 1.81 $mg.L^{-1}$.

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$:
$SRC_{eco, marine}$ = 1.81 $mg.L^{-1}$.

6.1.6 Aniline

The MPC derivation reported in sections 6.1.6.1 and 6.1.6.2 is based on the EU-RAR for aniline (EC, 2004a).

6.1.6.1 $MPC_{eco, water}$

The text in this section reflects the derivation presented in the EU-RAR.
Aquatic toxicity data for aniline can be found in Table A5. 6 (acute, freshwater) and Table A5. 24 (chronic, freshwater) in Appendix 5. Data used for ERL derivation are reported in Table A1. 6 in Appendix 1.

Freshwater

Chronic toxicity data for less than eight taxonomic groups are available. Therefore, the $MPC_{eco, water}$ is derived using preliminary effect assessment. Among the tested species *Daphnia* was most sensitive in both short-term and long-term tests. Therefore, the results from the *Daphnia* reproduction tests are used for the derivation of the $PNEC_{aqua}$.

In the EU-RAR for aniline, three valid 21-day NOECs of 4, 16 and 24 $\mu g.L^{-1}$ are reported for *Daphnia*. The NOEC of 4 $\mu g.L^{-1}$ derived from the study of Kühn *et al*. (1988, cited in EC, 2004a) is not as reliable as the other two daphnia tests, because this value was extrapolated from a nominal value of 10 $\mu g.L^{-1}$, based on the recovery rate that was determined at a much higher concentration. However, the decrease in test substance concentration of 40–60% is confirmed by the flow-though study of Hutton (1989, cited in EC, 2004a). Also in this test it was found that the measured concentrations were about 50% of the nominal values. In addition, the recovery rate of 40% does not take into account the possibly enhanced degradation of aniline in the presence of daphnid food. Therefore, the real NOEC may be lower than 4 $\mu g.L^{-1}$.
In the EU-RAR, the mean value of the three NOECs for *Daphnia* is calculated and used as basic value for the effect assessment. It was stated that the NOEC of 4 $\mu g.L^{-1}$ should be used for the derivation of the PNEC because it is possible that effects occur at concentrations below 4 $\mu g.L^{-1}$. As three *Daphnia* long-term tests are available that are regarded of equal value, it was considered to be most appropriate to use the arithmetic mean. Calculating the arithmetic mean of the three NOECs results in a value of 15 $\mu g.L^{-1}$ (the non-rounded off value was used in further calculations for INS purposes). For the derivation of the $PNEC_{aqua}$ an assessment factor of 10 was chosen, as reliable long-term tests are available for daphnids and fish. An effective NOEC on algae cannot be determined due to the rapid phototransformation of aniline in the presence of algae. However, as the nominal effect values from the algae tests are about 2-3 orders of magnitude higher than the NOECs from the *Daphnia* long-term tests, it can be expected with high probability that the effective algae NOEC is not below 15 $\mu g.L^{-1}$. Therefore: $PNEC_{aqua} = MPC_{eco,\ water}$ = 15 $\mu g.L^{-1}$ / 10 = 1.5 $\mu g.L^{-1}$.

Marine
No toxicity data for marine species were available from the EU-RAR for aniline. Therefore, an assessment factor of 100 is applied to the arithmetic mean of the three NOECs of *Daphnia* long-term tests. The $MPC_{eco,\ marine}$ = 15 $\mu g.L^{-1}$/ 100 = 0.15 $\mu g.L^{-1}$.

6.1.6.2 $MPC_{sp,\ water}$

According to the EU-RAR for aniline, the BCF of 2.6 L. kg^{-1} indicates that there is no bioaccumulation potential due to the exposure of organisms via water. Biomagnification via the food chain due to the route fish - fish-eating bird is not expected and an $MPC_{sp,\ water}$ is not determined. The same conclusion is drawn based on the trigger values discussed in sections 4.6.1 and 4.6.2 of this report.

6.1.6.3 $MPC_{hh\ food,\ water}$

The human toxicological threshold level for aniline (TL_{hh}) is a TDI of 0.00144 $mg.kg_{bw}^{-1}.d^{-1}$ (section 4.6.3). The TDI of 0.00144 $mg.kg_{bw}^{-1}.d^{-1}$ results in an $MPC_{hh,\ food}$ of 0.0877 $mg.kg_{fd}^{-1}$. The resulting $MPC_{hh\ food,\ water}$ is 0.0337 $mg.L^{-1}$ or 33.7 $\mu g.L^{-1}$.

6.1.6.4 $MPC_{dw,\ water}$

A provisional drinking-water standard is calculated, using the TDI of 0.00144 $mg.kg_{bw}^{-1}.d^{-1}$ as TL_{hh}. The resulting $MPC_{dw,\ water}$ is 0.00504 $mg.L^{-1}$ or 5.0 $\mu g.L^{-1}$.

6.1.6.5 Selection of the MPC_{water}

Freshwater
The following MPC_{water} were derived for aniline:
$MPC_{eco,\ water}$ = 1.5 $\mu g.L^{-1}$
$MPC_{hh\ food,\ water}$ = 34 $\mu g.L^{-1}$
$MPC_{dw,\ water}$ = 5.0 $\mu g.L^{-1}$

The $MPC_{eco, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for aniline is 1.5 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco, marine}$ =0.15 $\mu g.L^{-1}$
$MPC_{hh\ food, water}$ = 34 $\mu g.L^{-1}$

The lowest value is selected as MPC_{marine} values, which is the $MPC_{eco, water}$.
MPC_{marine} = 0.15 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

6.1.6.6 MAC_{eco}
For the derivation of the MAC_{eco}, an assessment factor of 100 is applied to the lowest EC50, because BCF < 100 $L.kg^{-1}$, log K_{ow} < 3 and the base set is complete. The lowest EC50 is found for *Daphnia pulex*: 0.1 $mg.L^{-1}$ from a study of Canton and Adema (1978, cited in EC, 2004a)
The resulting MAC_{eco} is 1.0 $\mu g.L^{-1}$.

6.1.6.7 SRC_{eco}
Freshwater
Since the base set is complete and NOECs for more than the three required taxa (alga, *Daphnia*, fish) are available, the SRC_{eco} is calculated as the geometric mean of all long term data. The resulting SRC_{eco} is 5.5 $mg.L^{-1}$.

Marine
The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$:
$SRC_{eco, marine}$ = 5.5 $mg.L^{-1}$.

6.1.7 Epichlorohydrin

6.1.7.1 $MPC_{eco, water}$
Since epichlorohydrin is vulnerable to volatilization and hydrolysis, only ecotoxicity data from experiments with suitable test systems were used for estimating MPCs:
- static test systems with closed bottles or test vessels and a short exposure period (maximum 24 h);
- static closed test systems but with chemical analysis of the tested concentration and a maximum exposure period of 72 h;
- closed test systems with renewal (semi-static) and/or chemical analysis;
- intermittent flow systems.

Aquatic toxicity data for epichlorohydrin can be found in Table A5. 7 (acute, freshwater), Table A5. 15 (acute, marine) and Table A5. 25 (chronic, freshwater) in Appendix 5. Data used for ERL derivation are reported in Table A1. 7 in Appendix 1.
Results of only one useful marine toxicity test are available: LC50s for a bacterium species. This marine data set is too small to investigate a potential difference in sensitivity of marine organism versus freshwater organisms to epichlorohydrin. Therefore, marine and freshwater data have been taken together for $MPC_{eco, water}$ derivation. Since toxicity data for less than eight taxonomic groups are available, the $MPC_{eco, water}$ is derived using preliminary effect assessment.

Freshwater
The base set is complete and the long-term NOECs do not fulfil the criteria to use them for the MPC derivation. Therefore, the $MPC_{eco, water}$ is based on the lowest acute test endpoint. The acute toxicity study for *Poecilia reticulata* (Deneer *et al.*, 1988) has the lowest value: LC50 = 0.65 $mg.L^{-1}$. This value (based on a 14 day closed renewal test) is much lower than the values from other tests with a shorter exposure period. For the whole group of chemicals tested by these authors, >50% of the substance originally added, was found back before renewal. No recovery percentage for epichlorohydrin itself was reported and the reported LC50s were based on the nominal values. Although the recovery value of >50% means that the true exposure concentrations for epichlorohydrin may have been somewhat lower than the nominal concentrations, the nominal LC50 of 0.65 $mg.L^{-1}$ is considered as a useable conservative estimate of the acute toxicity within the whole set of acute toxicity data for epichlorohydrin. Hence, the $MPC_{eco, water}$ is derived as 0.65 $mg.L^{-1}$ / 1000 = 0.65 $\mu g.L^{-1}$.

Marine
Since data for freshwater or marine representatives for at least three taxonomic groups (algae, crustaceans and fish) of three trophic levels are available, an assessment factor of 10000 is applied to the lowest value. Hence, the $MPC_{eco, marine}$ is 0.65 $mg.L^{-1}$ / 10000 = 0.065 $\mu g.L^{-1}$.

6.1.7.2 $MPC_{sp, water}$
Since epichlorohydrin has a log K_{ow} < 3, there is no potential for bioaccumulation. The assessment of secondary poisoning is not triggered, therefore a $MPC_{sp, water}$ is not derived.

6.1.7.3 $MPC_{hh\ food, water}$
Since epichlorohydrin is a probable carcinogen (R45), an $MPC_{hh\ food, water}$ should be derived. The human toxicological threshold level for epichlorohydrin (TL_{hh}) is 0.1 $\mu g.kg_{bw}^{-1}.d^{-1}$ (section 4.7.3). This risk limit is calculated into an $MPC_{hh, food}$ of 0.00609 $mg.kg_{fd}^{-1}$ using a BCF of 3.16 $L.kg^{-1}$ and a (default) BMF of 1. The resulting $MPC_{hh\ food, water}$ is 0.0019 $mg.L^{-1}$ or 1.90 $\mu g.L^{-1}$.

6.1.7.4 $MPC_{dw, water}$
A DW standard of 0.1 $\mu g.L^{-1}$ is available for epichlorohydrin, which is lower than the quality standards for other objectives of protection. Therefore a substance specific removal efficiency for drinking-water processing by simple treatment has to be identified. This treatment is defined as Category A1 in CD 75/44/EEC (EC, 1975) and consists of simple physical treatment (e.g. rapid filtration) and disinfection.

Due to its low K_{ow} value, epichlorohydrin is not expected to adsorb to a great extent onto DOC or POC, therefore, significant removal by coagulation and rapid filtration is not expected. The only remaining process by which epichlorohydrin can be removed is volatilization of the dissolved fraction by aeration. A removal efficiency of 4.6% was calculated for this process (based on the formulas in Zwolsman *et al.*, 2004), which means the fraction $F_{not\ removable\ by\ simple\ treatment}$ is 0.954. The $MPC_{dw, water}$ is then calculated as DW standard (CD 98/83/EC; EC, 1998) / $F_{not\ removable\ by\ simple\ treatment}$, which results in 0.10 / 0.954 = 0.10 $\mu g.L^{-1}$.

6.1.7.5 Selection of the MPC_{water}
Freshwater
The following MPC_{water} were derived for epichlorohydrin:
$MPC_{eco, water}$ = 0.65 $\mu g.L^{-1}$

$MPC_{hh\ food,\ water}$ = 1.90 µg.L^{-1}
$MPC_{dw,\ water}$ = 0.10 µg.L^{-1}

The $MPC_{dw,\ water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for epichlorohydrin is 0.10 µg.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco,\ marine}$ = 0.065 µg.L^{-1}
$MPC_{hh\ food,\ water}$ = 1.90 µg.L^{-1}

The MPC_{marine} is the lowest of the available MPC values. Hence MPC_{marine} = 0.065 µg.L^{-1} or 65 ng.L^{-1}. This value reflects the total fraction (see section 1.4.1).

6.1.7.6 MAC_{eco}

For the derivation of the MAC_{eco}, an assessment factor of 100 is applied to the lowest L(E)C50, because the base set is complete and log K_{ow} < 3 . The lowest LC50 is found for *Poecilia reticulata*: 0.65 mg.L^{-1} (650 µg.L^{-1}). The resulting MAC_{eco} is 0.0065 mg L^{-1} (6.5 µg.L^{-1}).

6.1.7.7 SRC_{eco}

Freshwater
Besides L(E)C50s, more than two NOECs are available, including a NOEC for one of the three specified taxa (i.e. algae). Since the geometric mean of the L(E)C50s/10 is lower than the geometric mean of the NOECs, the SRC_{eco} is calculated as the geometric mean of the L(E)C50s/10 = 3.1 mg.L^{-1} (3114 µg.L^{-1}).

Marine
The SRC_{eco} for the marine aquatic compartment, $SRC_{eco,\ marine}$, is set equal to the $SRC_{eco,\ water}$: $SRC_{eco,\ marine}$ = 3.1 mg.L^{-1}.

6.1.8 1,2-Dibromoethane

6.1.8.1 $MPC_{eco,\ water}$

Aquatic toxicity data for 1,2-dibromoethane can be found in Table A5. 8 (acute, freshwater), Table A5. 16 (acute, marine) and Table A5. 26 (chronic, freshwater) in Appendix 5. Data used for ERL derivation are reported in Table A1. 8 in Appendix 1.

Since the sensitivity of freshwater and marine organisms to 1,2-dibromoethane is not significantly different (P=0.56), the two datasets are combined for ERL derivation.

Freshwater
The base-set is complete and one chronic NOEC for fish is available. The lowest acute toxicity value is from the same trophic level as the NOEC, an assessment factor of 100 is applied to the NOEC for fish of 5.81 mg.L^{-1}. However, the lowest LC50 of 0.04 mg.L^{-1} was found for *Centropomus undecimalis*, while the NOEC of 5.81 mg.L^{-1} was determined for *Oryzias latipes*. In this case (LC50 and NOEC obtained for different species), the MPC should also be derived by application of an assessment factor of 1000 to the lowest LC50. This leads to an MPC of 0.04/1000 = 0.04 µg.L^{-1} or 40 ng.L^{-1}. The lowest value is selected and this results in an $MPC_{water,ecotox}$ of 0.04 µg.L^{-1} or 40 ng.L^{-1}.

Marine
No toxicity data for specific marine aquatic taxa are available for 1,2-dibromoethane. Therefore, an assessment factor of 10000 is applied to lowest L(E)C50 to derive the $MPC_{eco, marine}$.
The $MPC_{eco, marine}$ = 0.04 $mg.L^{-1}$/10000 = 0.004 $\mu g.L^{-1}$ or 4 $ng.L^{-1}$.

6.1.8.2 $MPC_{sp, water}$
Derivation of $MPC_{sp, water}$ for 1,2-dibromoethane is not triggered, since BCF < 100 and log K_{ow} < 3 (see section 4.11.2).

6.1.8.3 $MPC_{hh\ food, water}$
Since 1,2-dibromoethane is potentially carcinogenic (R45), $MPC_{hh\ food, water}$ should be derived. A BCF of 9.25 $L.kg^{-1}$ (see section 4.8.1) and a TL_{hh} of 5.0×10^{-7} $mg.kg_{bw}^{-1}.d^{-1}$ is used (see section 4.8.3). Using the equation from the INS guidance, the $MPC_{hh\ food, water}$ is 3.29 $ng.L^{-1}$.

6.1.8.4 $MPC_{dw, water}$
No A1 value and no DW standard are available. Therefore, a provisional drinking-water standard has to be calculated according to INS guidance. The TL_{hh} of 5.0×10^{-7} $mg.kg_{bw}^{-1}.d^{-1}$ is used and $MPC_{dw, water}$ is calculated to be 1.75 $ng.L^{-1}$.

6.1.8.5 Selection of the MPC_{water}
Freshwater
The following MPC_{water} values were derived for 1,2-dibromoethane:
$MPC_{eco, water}$ = 40 $ng.L^{-1}$
$MPC_{hh\ food, water}$ = 3.29 $ng.L^{-1}$
$MPC_{dw, water}$ = 1.75 $ng.L^{-1}$

The $MPC_{dw, water}$ is the lowest of the available MPC_{water} values. Therefore, the MPC_{water} for 1,2-dibromoethane is 1.75 $ng.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco, marine}$ = 0.004 $\mu g.L^{-1}$ or 4 $ng.L^{-1}$.
$MPC_{hh\ food, water}$ is 3.29 $ng.L^{-1}$

The $MPC_{hh\ food, water}$ is the lowest value of the available MPC_{marine} values. Therefore, the MPC_{marine} for methyl bromide is 3.29 $ng.L^{-1}$. This concentration reflects the total fraction.

6.1.8.6 MAC_{eco}
The base set is complete, BCF < 100 $L.kg^{-1}$and log K_{ow} < 3. Therefore an assessment factor of 100 is applied to the lowest EC50 to derive the MAC_{eco}. The lowest EC50 is found for *Centropomus undecimalis* and is 0.04 $mg.L^{-1}$. The resulting MAC_{eco} is 0.4 $\mu g.L^{-1}$.

6.1.8.7 SRC_{eco}
Freshwater
Since there is one NOEC available for fish and the geometric mean of the L(E)C50 /10 is lower than the NOEC value, the SRC_{eco} is based on the geometric mean of the L(E)C50s with an assessment factor of 10. This results in an SRC_{eco} of 0.79 $mg.L^{-1}$.

Marine
The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine} = 0.79$ mg.L^{-1}.

6.1.9 Ethinylestradiol

6.1.9.1 $MPC_{eco, water}$

Aquatic toxicity data for ethinylestradiol can be found in Table A5. 9 (acute, freshwater), Table A5. 17 (acute, marine), Table A5. 27 (chronic, freshwater) and Table A5. 32 (chronic, marine) in Appendix 5. Data used for ERL derivation are reported in Table A1. 9 in Appendix 1.
Acute toxicity data were found for both freshwater organisms (algae, crustaceans and cnidarians) and saltwater organisms (crustaceans and echinoderms). Chronic toxicity data were also found for freshwater (algae, molluscs, crustaceans, fish and rotifers) and saltwater organisms (crustaceans and fish).
Chronic data were log normally distributed. However, fish were clearly the most sensitive taxon to ethinylestradiol exposure, because all fish data were concentrated in the left tail of the distribution. It has to be noted that amphibians may be sensitive as well. Park and Kidd (2005) showed effects on the hatching rate of green frogs (*Rana clamitans*) in a field study at 5 ng.L^{-1}. Recent information on chronic toxicity to amphibians (*Xenopus tropicalis*) is given by Petterson *et al*. (2006), but unfortunately a NOEC for the endpoint sex ratio was not determined since the lowest test concentration (*viz*. 300 ng.L^{-1}) already showed effect. Short term toxicity focusing on lethality as endpoint did not show enhanced sensitivity (Hogan *et al.*, 2006).
Since fish were observed to be extremely sensitive to ethinylestradiol exposure, when compared to other taxa, only chronic toxicity data for freshwater and marine fish were compared for sensitivity. Data on similar endpoints for the same species were not pooled, because the underlying experiments were started at different life stages (e.g. eggs vs. adults). The sensitivity of chronic freshwater and marine organisms to ethinylestradiol was not significantly different (p=0.90), although it must be noted that the marine data set is very small compared to the freshwater data set, making the comparison less meaningful. All chronic data were combined to one data set for ERL derivation.

Freshwater
The base set is complete, the MPC will be derived using assessment factors. The derivation of the MPC is based on the $NOEC_{fertillisation}$ of 0.16 ng.L^{-1} for *Pimephales promelas* (Parrott and Blunt, 2005). Using an assessment factor of 10, this results in a freshwater $MPC_{eco, water}$ of 0.016 ng.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).It has to be noted that this value is below the detection limit of ethinylestradiol, which is reported to be 0.74-1.5 ng.L^{-1} (Parrott and Blunt, 2005), 0.1-2.4 ng.L^{-1} (Belfroid *et al.*, 1999) or 0.02-1.3 ng.L^{-1} (ARCEM, 2003). Young *et al*. (2002) determined a PNEC of 0.1 ng.L^{-1} based on an MATC (maximum acceptable toxicant concentration) of 0.57 ng.L^{-1} for *Danio rerio* and an assessment factor of 5. ARCEM (Austrian research cooperation on endocrine modulators) also suggested a PNEC of 0.1 ng.L^{-1}, based on a NOEC of 1 ng.L^{-1} for *Pimephales promelas*, as determined by Länge *et al*. (2001).

Both PNECs of 0.1 ng.L^{-1} are a factor of 6 higher than the $MPC_{eco, water}$ derived in this report. The lower MPC derived here is caused by the availability of a more recent study (Parrot and Blunt). A slightly higher sensitivity of *P. promelas* towards ethinylestradiol was found compared to previously reported values. This result, combined with an assessment factor of 10 lead to the lower value presented in our report. Since toxicity data for other potentially sensitive groups of organisms are absent (e.g. gastropods) or limited (e.g. amphibians; two NOECs < 300 ng.L^{-1} available ;

Petterson *et al*., 2006) and a NOEC <0.1 ng.L^{-1} for *P. promelas* (Jobling *et al.*, 2004) is reported, the assessment factor of 10 is deemed justified.
Marine
Using an assessment factor of 100 on the $NOEC_{fertillisation}$ of 0.16 ng.L^{-1} for *Pimephales promelas* results in an $MPC_{eco, marine}$ of 0.0016 ng.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).

6.1.9.2 $MPC_{sp, water}$

Freshwater
No useful toxicity data for birds or mammals were found. A NOAEL of 3 µg.kg_{bw}^{-1}.d^{-1} was available for estradiol from a chronic 90 day study with rats (JECFA, 2000). A factor of 50 is proposed to compensate for the higher estrogenic potential of ethinylestradiol in humans (see section 4.9.3). Assuming that this ratio is similar in mammals (and birds), the $NOAEL_{rat}$ of 3 µg.kg_{bw}^{-1}.d^{-1} for estradiol can be extrapolated to 0.06 µg.kg_{bw}^{-1}.d^{-1} for ethinylestradiol. Conversion to a concentration in food using a factor of 20 (TGD and INS guidance) results in a $NOEC_{rat}$ of 1.2 µg.kg_{fd}^{-1}. Applying an assessment factor of 90, this NOEC results in an $MPC_{oral, mammal}$ (= $MPC_{oral, min}$) of 13.3 ng.kg_{fd}^{-1}. Subsequently, using a BCF_{fish} of 263 (QSAR) and a BMF_1 of 1, results in an $MPC_{sp, water}$ of 0.0507 ng.L^{-1}.

Marine
Since BMF_2 for ethinylestradiol is 1 by default, the $MPC_{marine, sp}$ for the marine environment is also equal to 0.0507 ng.L^{-1}.

6.1.9.3 $MPC_{hh\ food, water}$

Since ethinylestradiol is labelled as a class 1 carcinogenic, as stated in IARC monograph Vol. 21 (IARC, 1979) and Suppl. 7 (IARC, 1987b) and its log K_{ow} is ≥ 3, an $MPC_{hh\ food, water}$ is derived. Based on a TL_{hh} of 1 ng.kg_{bw}^{-1}.d^{-1}, an $MPC_{hh\ food, water}$ of 0.23 ng.L^{-1} is calculated.

6.1.9.4 $MPC_{dw, water}$

Based on a TL_{hh} of 1 ng.kg_{bw}^{-1}.d^{-1}, an $MPC_{dw, water}$ of 3.5 ng.L^{-1} is calculated.

6.1.9.5 Selection of the MPC_{water}

Freshwater
The following MPC_{water} values were derived for ethinylestradiol:
$MPC_{eco, water}$ = 0.016 ng.L^{-1}
$MPC_{sp, water}$ = 0.051 ng.L^{-1}
$MPC_{hh\ food, water}$ = 0.23 ng.L^{-1}
$MPC_{dw, water}$ = 3.5 ng.L^{-1}

The $MPC_{eco, water}$ is the lowest of the available MPC_{water} values. Therefore the MPC_{water} for ethinylestradiol is 0.016 ng.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco, marine}$ = 0.0016 ng.L^{-1}
$MPC_{marine, sp}$ = 0.051 ng.L^{-1}
$MPC_{hh\ food, water}$ is 0.23 ng.L^{-1}

The $MPC_{eco, marine}$ is the lowest value of the available MPC_{marine} values. Therefore, the MPC_{marine} for ethinylestradiol is 0.0016 $ng.L^{-1}$ or 1.6 $pg.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

6.1.9.6 MAC_{eco}

Because the base set is complete and ethinylestradiol is potentially bioaccumulative, an assessment factor of 1000 is applied to the lowest $L(E)C_{50}$ of 0.56 $mg.L^{-1}$ (for the amphibian *Rana sylvatica*). This yields a MAC_{eco} value of 0.56 $\mu g.L^{-1}$.

6.1.9.7 SRC_{eco}

Freshwater

Chronic toxicity data for six taxonomic groups are available. Following INS guidance, the SRC_{eco} should be derived using both chronic freshwater and marine ecotoxicity data and calculated by taking the geometric mean of these data. The resulting value is 0.50 $\mu g.L^{-1}$. However, since fish appear to be the most sensitive taxon (all data located in the left tail of the distribution), the calculated SRC_{eco} would greatly underestimate serious risks for this group of organisms. Therefore, the SRC_{eco} is based on the geometric mean of the chronic fish data. This results in an SRC_{eco} of 2.43 $ng.L^{-1}$ (90% CI 0.23 – 26 $ng.L^{-1}$).

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine}$ = 2.43 $ng.L^{-1}$.

6.1.10 Methyl bromide

6.1.10.1 $MPC_{eco, water}$

Aquatic toxicity data for methyl bromide can be found in Table A5. 10 (acute, freshwater) and Table A5. 28 (chronic, freshwater) in Appendix 5. Data used for ERL derivation are reported in Table A1. 10 in Appendix 1.

Freshwater

The base set is complete. Data for three trophic levels are present, represented by algae, *Daphnia* and fish. Chronic data are available for one trophic level: secondary consumers, represented by fish. The available chronic NOEC is from the same trophic level as that of the lowest acute LC50. Moreover, the species for which the NOEC is determined is the same species as that for which the lowest LC50 was found (viz. *Oryzias latipes*). Therefore, an assessment factor of 100 is applied to the lowest NOEC of 0.32 $mg.L^{-1}$. The $MPC_{eco, water}$ is 0.32/100=0.0032 $mg.L^{-1}$ or 3.2 $\mu g.L^{-1}$.

Marine

No data on specific marine taxa are available. The MPC_{marine} is derived from the chronic study with *Oryzias latipes* and an assessment factor of 1000. MPC_{marine} = 0.32 $mg.L^{-1}$ /1000 = 0.32 $\mu g.L^{-1}$.

6.1.10.2 $MPC_{sp, water}$

Derivation of $MPC_{sp, water}$ for methyl bromide is not triggered. BCF < 100 and log K_{ow} < 3 (see section 4.11.2).

6.1.10.3 $MPC_{hh\ food, water}$

Derivation of $MPC_{hh\ food, water}$ for methyl bromide is not triggered (see section 4.11.2).

6.1.10.4 $MPC_{dw, water}$

A provisional drinking-water standard has to be calculated according to the equation provided in INS guidance. The TL_{hh} used for $MPC_{dw, water}$ derivation is the RfD of 1.40×10^{-3} $mg.kg_{bw}^{-1}.d^{-1}$ (see section 4.10.3). $MPC_{dw, water} = 4.9$ $\mu g.L^{-1}$.

6.1.10.5 Selection of the MPC_{water}

The following MPC_{water} values were derived for methyl bromide:
$MPC_{eco, water} = 3.2$ $\mu g.L^{-1}$
$MPC_{dw, water} = 4.9$ $\mu g.L^{-1}$

The $MPC_{eco, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for methyl bromide is 3.2 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment the following MPCs were determined:
$MPC_{eco, marine} = 0.32$ $\mu g.L^{-1}$

The MPC_{marine} is set equal to the $MPC_{eco, marine} = 0.32$ $\mu g.L^{-1}$. This concentration reflects the total fraction.

6.1.10.6 MAC_{eco}

For the derivation of the MAC_{eco}, an assessment factor of 100 is applied to the lowest EC50, because the base set is complete, BCF < 100 $L.kg^{-1}$ and log K_{ow} < 3. The lowest EC50 is found for *Oryzias latipes* (0.7 $mg.L^{-1}$), in a study of Canton *et al.* (1980). The resulting MAC_{eco} is 7 $\mu g.L^{-1}$.

6.1.10.7 SRC_{eco}

Freshwater
Since there are two NOECs available for fish and the geometric mean of the L(E)C50s/10 is higher than the geometric mean of the NOECs, the SRC_{eco} is based on the geometric mean of the available NOECs. This results in an SRC_{eco} of 0.179 $mg.L^{-1}$.

Marine
The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$:
$SRC_{eco, marine} = 0.179$ $mg.L^{-1}$.

6.1.11 6PPD

6.1.11.1 $MPC_{eco, water}$

Aquatic toxicity data for 6PPD can be found in Table A5. 11 (acute, freshwater), Table A5. 29 (chronic, freshwater) and (chronic, marine) in Appendix 5. Data used for ERL derivation are reported in Table A1. 11 in Appendix 1.

Since 6PPD is unstable in aerobic water at neutral or basic pH, results from toxicity tests without analytically monitored concentrations should be interpreted with care. Study information from IUCLID entries was lacking detailed information on toxicity studies. These were therefore considered not useful. A 'robust summary' from US EPA's HPV Challenge Program was retrieved, which contained detailed information on some of the IUCLID entries (US EPA, 2003). Acute results for *Daphnia* from this US EPA report were used provided concentrations were monitored. Two of the original study reports sponsored by Monsanto and summarised in both the IUCLID and

US EPA reports, were retrieved, evaluated and used for ERL derivation. An EC50 and EC10 for *Pseudokirchneriella subcapitata* as well as an 4 day LC50 and a 28 day NOEC (mortality) for *Pimephales promelas* were obtained from these study reports. More studies that could be used in ERL derivation were not encountered.

The highest half-life values for 6PPD reported in water are approximately 1 day (pure or deionised water), whereas the lowest half-life values are 3 to 7 hours (algal medium, pH 7 buffered water, river water). This implicates that in all static and most renewal tests with 6PPD, the test organism will have been exposed to a mixture of 6PPD and degradation products. E.g. in a standard acute (48 h) *Daphnia* toxicity test, the test water is not renewed, meaning that the one valid test result for *Daphnia magna* (EC50 0.23 $mg.L^{-1}$), in fact reflects exposure to 6PPD *plus* metabolites even though the EC50 is expressed as a 6PPD concentration.

For the crustacean species *Daphnia magna*, the 48 hour EC50 of a solution aged 24 hours before onset of the toxicity test was less toxic than when Daphnids were exposed to spiked solution immediately. Concentrations were analytically determined in this test. Thus, 6PPD seems to be more toxic to *D. magna* than its degradation products. Test results from other acute studies with *D. magna* based on nominal concentrations are in the same range as the EC50 from the test described earlier (0.51 $mg.L^{-1}$). This implies that the EC50 from the test with actual concentrations is most likely based on nominal concentrations (this was not reported).

The results from the algal toxicity test in Table A5. 11 and Table A5. 29 is based on nominal concentrations and the EC50 and EC10 should therefore be considered as less reliable. Toxicity exhibited during 96 hours was also determined by degradation products of 6PPD. However, using the information that degradation products of 6PPD were less toxic than the parent compound to *Daphnia* (see previous section), the EC50 and EC10 for *Pseudokirchneriella subcapitata* are not expected to be much lower than the values obtained in the algal toxicity study.

Description of key study: Thompson *et al*., (1979)
A chronic study with the fish *Pimephales promelas* was performed. The study was an intermittent flow study with analytical monitoring of 6PPD with 30 fish per aquarium. Five concentrations plus a control were tested: control, 66, 120, 230, 450 and 1000 $\mu g.L^{-1}$ (nominal concentrations). A 4 day LC50 as well as a 28 day NOEC can be obtained from this study. The test was performed under acceptable conditions; dead animals were removed, pH and O_2 were well within acceptable levels throughout the test. The 4 day LC50 (0.45 $mg.L^{-1}$) was determined by the authors, who also reported a 28 day LC50. Since the latter value is not useful for ERL derivation, the original data were used to obtain a NOEC. At day 28, cumulative mortality in the six treatments was as follows (treatments in increasing order): 0% (control), 0%, 20%, 100%, 100%, 100%. The lowest treatment (nominal: 66 $\mu g.L^{-1}$) was selected as NOEC. The authors have based their final LC50 on nominal concentrations since they reported a decrease in mean measured concentrations that could not be explained. In this report, we will base the NOEC on the mean measured concentration because of the following reasons.

The recovery of the analytical method was verified at each sampling time (at 7 days during the test) and proved to be more or less stable: 67%-100%. Mean measured values were always corrected for recovery determined at the specific sampling day. The overall mean of measured concentrations revealed that the lower 6PPD treatments appeared to decline most strongly in 6PPD concentration. Authors could not satisfactorily explain this phenomenon and proposed to use the nominal concentration, but put forward the possibility of degradation. In addition to chemical degradation, it is the raw data suggest that metabolism of 6PPD by (surviving) fish contributes to the concentration

decrease observed during the test. It is proposed here to use the mean measured concentrations to report the outcome of this test: NOEC for mortality is 24 $\mu g.L^{-1}$. It should be kept in mind, that this NOEC reflects mortality of 6PPD and its degradation products.

Freshwater
Based on the argumentation outlined above, the base set for acute toxicity is accepted as complete. Data for three trophic levels are present, represented by algae, *Daphnia* and fish. Chronic data for two trophic levels are available: primary producers and secondary consumers, represented by algae and fish. This dataset allows for application of an assessment factor of 50 to the lowest NOEC. Note that the lowest LC50 is in the same range as the NOEC: 0.028 $mg.L^{-1}$ vs. 0.024 $mg.L^{-1}$. If the lowest LC50 would have been lower than the lowest NOEC, an assessment factor of 100 should have been applied to the LC50 (EU-TGD guidance), which would have resulted in a lower MPC. Based on the chronic test, the $MPC_{eco, water}$ is derived as 24/50 = 0.48 $\mu g.L^{-1}$.

Marine
No toxicity data for marine aquatic species were available for 6PPD. Therefore, an assessment factor of 500 is applied to lowest NOEC to derive the $MPC_{eco, marine}$.
The $MPC_{eco, marine}$ = 0.024/500 = 0.000048 $mg.L^{-1}$ or 0.048 $\mu g.L^{-1}$.

6.1.11.2 $MPC_{sp, water}$
Derivation of $MPC_{sp, water}$ for 6PPD is not triggered (see section 4.11.2).

6.1.11.3 $MPC_{hh\ food, water}$
Derivation of $MPC_{hh\ food, water}$ for 6PPD is not triggered (see section 4.11.2).

6.1.11.4 $MPC_{dw, water}$
A provisional drinking-water standard is calculated, using the TL_{hh} of 0.75 $mg.kg_{bw}^{-1}.d^{-1}$ (see section 4.11.3). The resulting $MPC_{dw, water}$ is 2.63 $mg.L^{-1}$.

6.1.11.5 Selection of the MPC_{water}
Freshwater
The following MPC_{water} were derived for 6PPD:
$MPC_{eco, water}$ = 0.48 $\mu g.L^{-1}$
$MPC_{dw, water}$ = 2630 $\mu g.L^{-1}$

The $MPC_{eco, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for 6PPD is 0.48 $\mu g.L^{-1}$. This concentration reflects the total fraction (see section 1.4.1).

Marine
For the marine environment only one MPC is determined: $MPC_{eco, marine}$ = 0.048 $\mu g.L^{-1}$. This value is selected as MPC_{marine}. This concentration reflects the total fraction (see section 1.4.1).

6.1.11.6 MAC_{eco}
6PPD has no bioaccumulation potential. The mode of action of 6PPD is not known, however, interspecies variation is not considered to be low: the range of acute toxicity test results spans a factor of 30. An assessment factor of 100 is applied to the lowest acute test result (LC50 of 28 $\mu g.L^{-1}$ for *O. latipes*) to derive the MAC_{eco}. MAC_{eco} = 28/100 = 0.28 $\mu g.L^{-1}$.

6.1.11.7 SRC_{eco}

Freshwater

Since the geometric mean of the L(E)C50s/10 is lower than the geometric mean of the two available NOECs, the SRC_{eco} is based on the L(E)C50s. This results in an SRC_{eco} of 21 $\mu g.L^{-1}$.

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine}$ = 21 $\mu g.L^{-1}$.

6.1.12 DCB

6.1.12.1 $MPC_{eco, water}$

Aquatic toxicity data for DCB can be found in Table A5. 12 (acute, freshwater), Table A5. 18 (acute, marine) and Table A5. 30 (chronic, freshwater) in Appendix 5. Data used for ERL derivation are reported in Table A1. 12 in Appendix 1.
Two useful marine toxicity test results are available: an LC50 for a bacterium and for a fish species. This marine data set is considered too small to investigate a potential difference in sensitivity of marine organism versus freshwater organisms to DCB. Therefore, marine and freshwater data have been taken together for $MPC_{eco, water}$ derivation.

Freshwater

The base-set is complete and one chronic test result is available. Since the single available chronic test result is for an algal species, an assessment factor of 1000 should be applied to the lowest acute L(E)C50 value, which is the EC50 for the bacterium *Vibrio fischeri*.
The $MPC_{eco, water}$ is therefore 0.058 $mg.L^{-1}$/1000 = 0.058 $\mu g.L^{-1}$ or 58 $ng.L^{-1}$.

Marine

No toxicity data for specific marine aquatic taxa are available for DCB. Therefore, an assessment factor of 10000 is applied to lowest L(E)C50 to derive the $MPC_{eco, marine}$.
The $MPC_{eco, marine}$ = 0.058 $mg.L^{-1}$/10000 = 0.0058 $\mu g.L^{-1}$ or 5.8 $ng.L^{-1}$.

6.1.12.2 $MPC_{sp, water}$

The $NOEC_{mammal, food\ chr}$ derived for DCB is 40 $mg.kg_{fd}^{-1}$ (see section 4.12.4). Since this value is based on a NOAEL from a chronic study, an assessment factor of 30 is applied (TGD and INS guidance) to calculate the $MPC_{oral, mammal}$. This results in an $MPC_{oral, mammal}$ of 1.33 $mg.kg_{fd}^{-1}$. Using the BCF of 501 $L.kg^{-1}$ and a BMF_1 of 1, the $MPC_{sp, water}$ becomes 0.00266 $mg.L^{-1}$ or 2.66 $\mu g.L^{-1}$.

Marine

Since the BMF_2 is also 1, the marine $MPC_{marine, sp}$ is equal to the $MPC_{sp, water}$ for freshwater.

6.1.12.3 $MPC_{hh\ food, water}$

Freshwater

Since DCB is potentially carcinogenic (R45), $MPC_{hh\ food, water}$ should be derived. The BCF of 501 $L.kg^{-1}$ (see section 4.12.1) and the TL_{hh} of 0.0043 $ng.kg_{bw}^{-1}.d^{-1}$ are used (see section 4.12.3). Using the equations and defaults from INS guidance, $MPC_{hh, food}$ = 2.61 $ng.kg_{fd}^{-1}$.
The resulting $MPC_{hh\ food, water}$ is 0.0052 $ng.L^{-1}$ or 5.2 $pg.L^{-1}$.

6.1.12.4 $MPC_{dw, water}$

The $MPC_{dw, water}$ is calculated using the TL_{hh} of 0.0043 $ng.kg_{bw}^{-1}.d^{-1}$ and the equation and defaults from INS guidance. The resulting $MPC_{dw, water}$ = 0.15 $ng.L^{-1}$.

6.1.12.5 Selection of the MPC_{water}

Freshwater

The following MPC_{water} were derived for DCB:
$MPC_{eco, water}$ = 58 ng.L^{-1}
$MPC_{sp, water}$ = 2660 ng.L^{-1}
$MPC_{hh\ food, water}$ is 0.0052 ng.L^{-1}
$MPC_{dw, water}$ = 0.15 ng.L^{-1}

The $MPC_{hh\ food, water}$ is the lowest of the available MPC_{water} values. Therefore, MPC_{water} for DCB is 5.2 pg.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).

Marine

The following MPCs were derived for the marine compartment:
$MPC_{eco, marine}$ = 5.8 ng.L^{-1}
$MPC_{marine, sp}$ = 2660 ng.L^{-1}
$MPC_{hh\ food, water}$ is 0.0052 ng.L^{-1}

The MPC_{marine} will be set equal to the lowest value of the available MPC values, which is $MPC_{hh\ food, water}$. Therefore, MPC_{marine} for DCB is 0.0052 ng.L^{-1} or 5.2 pg.L^{-1}. This concentration reflects the total fraction (see section 1.4.1).

6.1.12.6 MAC_{eco}

Since the base set is complete for DCB and there is a potential to bioaccumulate (BCF = 501 L.kg^{-1}), an assessment factor of 1000 should be applied to the lowest L(E)C50. This results in a MAC_{eco} of 0.058 mg.L^{-1} /1000 = 0.058 µg.L^{-1} or 58 ng.L^{-1}.

6.1.12.7 SRC_{eco}

Freshwater

The geometric mean of acute toxicity data, divided by an assessment factor of 10 is 0.096 mg.L^{-1}. One NOEC value of 0.32 mg.L^{-1} is available. Since the use of acute toxicity data leads to the lowest value, this value is selected as SRC. The $SRC_{eco, water}$ is thus equal to 0.096 mg.L^{-1} = 96 µg.L^{-1}.

Marine

The SRC_{eco} for the marine aquatic compartment, $SRC_{eco, marine}$, is set equal to the $SRC_{eco, water}$: $SRC_{eco, marine}$ = 96 µg.L^{-1}.

7. Toxicity data and derivation of ERLs for soil and sediment

7.1 ERL derivation for soil

7.1.1 PentaBDE

7.1.1.1 MPC

Direct (eco)toxicity in soil

The MPC_{soil} derivation for pentaBDE is cited from the EU-RAR (EC, 2001). Toxicity data of pentaBDE to terrestrial organisms are shown in Table A6. 1 (acute) and Table A6. 5 (chronic) in Appendix 6. In the EU-RAR, the $PNEC_{soil}$ was derived by applying an assessment factor of 50 to the NOEC of 16 $mg.kg^{-1}$ for toxicity to emergence of *Zea mays*, resulting in a PNEC of 0.38 $mg.kg_{dw}^{-1}$ EU standard soil. Converting this value to Dutch characteristics gives an MPC_{soil} of 1.1 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning

The human toxicological standard published by De Winter-Sorkina *et al*. (2006) is used for the derivation of the $MPC_{oral, min}$. The $MPC_{oral, min}$ is derived in section 6.1.1.2 for secondary poisoning in the aquatic compartment. This value is also used for calculation of secondary poisoning in soil. The $MPC_{oral, min}$ is 13.3 $\mu g.kg_{fd}^{-1}$. $BCF_{earthworm}$ is calculated using the TGD QSAR and the selected log K_{ow} of 6.57, resulting in a value of 44585 $L.kg_{wwt}^{-1}$. Further input for the calculation of $MPC_{soil, sp}$ are the selected values for log K_{oc} = 5.75 $L.kg^{-1}$ and H = 23.4 $Pa.m^3.mol^{-1}$. Using the equation presented in INS guidance (which is derived from TGD guidance), the calculated $MPC_{soil, sp}$ = 10.7 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$

Of the four human exposure routes considered, consumption of meat (cows) is the most critical route. The $MPC_{human, soil}$ based on this route is 4.31×10^{-7} $mg.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}

The lowest of the three derived MPC_{soil} values is selected, which is the $MPC_{human, soil}$. Hence, MPC_{soil} is 4.3×10^{-7} $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.1.2 SRC_{eco}

Since two NOEC values are available (for one terrestrial plant species), the SRC_{eco} is calculated as the geometric mean of these NOEC. The resulting SRC_{eco} is 154 $mg.kg_{dw}^{-1}$ Dutch standard soil.

It should be noted that since a complete overview of all relevant toxicity studies for birds and mammals is not available from the data sources used for ERL derivation (WFD fact sheet and EU-RAR), a geometric mean of all $MPC_{oral, min}$ values can not be derived. This hampers derivation of an SRC_{eco} based on secondary poisoning.

7.1.2 p-*tert*-octylphenol

7.1.2.1 MPC

Direct ecotoxicity - equilibrium partitioning

The report by the UK environment agency (Brooke *et al.*, 2005), which is the basis for this ERL derivation, states that no data on toxicity of p-*tert*-octylphenol to terrestrial organisms were available. The MPC_{soil} is therefore calculated using EqP. To that end, the $MPC_{eco, water}$ of 0.122 $\mu g.L^{-1}$ and a log K_{oc} of 3.43 were used, together with the characteristics of Dutch standard soil. This results in an MPC_{soil} of 19.4 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning

The $MPC_{oral, min}$ derived in section 6.1.2.2 for secondary poisoning in the aquatic compartment is used for calculation of secondary poisoning in soil as well. The $MPC_{oral, min}$ is 10 $mg.kg_{fd}^{-1}$. $BCF_{earthworm}$ is calculated using the TGD QSAR and the selected log K_{ow} of 4.12, resulting in a value of 159 $L.kg_{wwt}^{-1}$. Further input for the calculation of $MPC_{soil, sp}$ are the selected values for log K_{oc} = 3.43 $L.kg^{-1}$ and H = 0.52 $Pa.m^3.mol^{-1}$. Using the equation presented in INS guidance (which is derived from TGD guidance), the calculated $MPC_{soil, sp}$ = 10.7 $mg.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$

Of the four human exposure routes considered, consumption of root crops is the most critical route. The $MPC_{human, soil}$ based on this route is 2.29 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}

The lowest of the three derived MPC_{soil} values is selected, which is the MPC_{soil} based on equilibrium partitioning. Hence, MPC_{soil} is 19.4 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.2.2 SRC_{eco}

The SRC_{eco} for soil is calculated using EqP, based on the SRC_{eco} for water. The following values were used: $SRC_{eco, water}$ = 40.8 $\mu g.L^{-1}$ and log K_{oc} = 3.43. The resulting SRC_{eco} for soil is 6.47 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Note. Since a complete overview of all relevant toxicity studies for birds and mammals is not available from the data sources used for ERL derivation (Brooke *et al.*, 2005), a geometric mean of all $MPC_{oral, min}$ values can not be derived. This hampers derivation of an SRC_{eco} based on secondary poisoning.

7.1.3 Benzo[*b*]fluoranthene

7.1.3.1 MPC

Direct ecotoxicity - equilibrium partitioning

The MPC_{soil} derivation for benzo[*b*]fluoranthene is cited from the draft EU-RAR on coal tar pitch (EC, 2006b). Toxicity data of benzo[*b*]fluoranthene to terrestrial organisms are shown in Table A6. 6 (chronic) in Appendix 6.

Citation from draft EU-RAR on PCTHT (EC, 2006b):
'The only toxicity study with terrestrial species for benzo[*b*]fluoranthene is a 21 day study with *Folsomia fimetaria* (Sverdrup *et al*., 2002, cited in EC, 2006b). Up to concentrations of 450 $mg.kg_{dw}^{-1}$ (recalculated to a soil with 2% organic carbon) no effects were observed. The PNEC for soil has to be derived by equilibrium partitioning, resulting in a value of 0.28 mg/kg_{dw}.'

Since no effect concentration was established, this toxicity result can not be used to derive an MPC. Hence, terrestrial toxicity data are not available for benzo[*b*]fluoranthene. Since a read across was performed with benzo[*k*]fluoranthene for the derivation of the $MPC_{eco, water}$, terrestrial toxicity data for benzo[*k*]fluoranthene have been taken into consideration as well. Toxicity data of benzo[*b*]fluoranthene to terrestrial organisms are shown in Table A6. 7 in Appendix 6.
Citation from draft EU-RAR on PCTHT (EC, 2006b):
'The only toxicity studies with terrestrial species for benzo[*k*]fluoranthene are a 21-d study with *Folsomia candida* (Bowmer *et al*., 1993, cited in EC, 2006b) and a 21-d study with *Folsomia fimetaria* (Sverdrup *et al*., 2002, cited in EC, 2006b). Up to concentrations of 61 mg/kg_{dw}, recalculated to a soil with 2% organic carbon, no effects were observed for *F. candida*. For *F. fimetaria* this concentration was 710 mg/kg_{dw}.'

For both benzo[*b*]fluoranthene and benzo[*k*]fluoranthene the available studies did not result in endpoints useful for MPC derivation. Therefore, the PNEC for soil had to be derived by equilibrium partitioning. Using $MPC_{eco, water}$ = 0.017 $\mu g.L^{-1}$, log K_{oc} = 5.91 and H = 0.051 $Pa.m^3.mol^{-1}$, this results in a PNEC of 0.28 $mg.kg_{dw}^{-1}$ EU standard soil. This is equal to 0.813 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning
Since a $PNEC_{oral}$ has not been derived in the draft EU-RAR on coal tar pitch, risk limits based on secondary poisoning ($MPC_{sp, soil}$) can not be derived.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of leafy crops is the most critical route. The $MPC_{human, soil}$ based on this route is 0.40 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the $MPC_{human, soil}$. Hence, MPC_{soil} is 0.40 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.3.2 SRC_{eco}
The SRC_{eco} for soil is calculated using EqP, based on the SRC_{eco} for water. The following values were used: $SRC_{eco, water}$ = 0.17 $\mu g.L^{-1}$, log K_{oc} = 5.91 and H = 0.051 $Pa.m^3.mol^{-1}$. The resulting $SRC_{eco, soil}$ is 8.3 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.4 Isodrin
No toxicity data or physicochemical data have been collected for isodrin. For this reason, an MPC or SRC_{eco} for soil are not derived.

7.1.5 DNOC
7.1.5.1 MPC
Direct (eco)toxicity in soil
The toxicity data of DNOC to terrestrial organisms are shown in Table A6. 2 (chronic) and Table A6. 10 (microbial processes and enzymatic reactions) in Appendix 6. Since more than one toxicity test result for a terrestrial organism is available, the MPC_{soil} should be derived on the basis of the terrestrial toxicity data. Two LC50s are available (earthworms) and two NOECs (microbial

processes and enzymatic activity). An assessment factor of 100 is applied to the lowest NOEC, to derive the MPC_{soil}. MPC_{soil} = 16.9/100 = 0.17 $mg.kg_{dw}^{-1}$ Dutch standard soil.

The height of the available LC50s (earthworm) is 65 and 20 $mg.kg^{-1}$, respectively, which is in the same range as the NOEC for enzymatic activity of 17 $mg.kg^{-1}$. Since the lowest LC50 is actually derived from a chronic test (duration 28 d), an assessment factor of 100 seems justified.
Deriving an MPC_{soil} using EqP is not necessary following INS guidance. However, the amount of toxicity data for soil species is very small and does not adequately represent the terrestrial ecosystem. A calculation of the MPC_{soil} using EqP ($MPC_{eco, water}$ = 9.2 $\mu g.L^{-1}$, log K_{oc} = 2.75) results in a value of 0.30 $mg.kg_{dw}^{-1}$ standard soil. Although the EqP-based value will not be used to set the MPC, it adds some confidence to the height of the MPC_{soil} based on terrestrial toxicity data, since both values are in the same order of magnitude.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of leafy crops is the most critical route. The $MPC_{human, soil}$ based on this route is 0.38 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the MPC_{soil} based on ecotoxicological data for soil organisms. Hence, MPC_{soil} is 0.17 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.5.2 SRC_{eco}
The SRC_{eco} for DNOC is derived both on the basis of the terrestrial chronic toxicity data and on the basis of the chronic aquatic toxicity data (using EqP), since only chronic (terrestrial) data for one trophic level is available.
$SRC_{eco, direct}$ = 19.5 $mg.kg^{-1}$ standard soil and $SRC_{eco, EqP}$ = 60.1 $mg.kg^{-1}$ Dutch standard soil. The lowest value is selected, therefore SRC_{eco} = 19.5 $mg.kg^{-1}$ Dutch standard soil.

7.1.6 Aniline

7.1.6.1 MPC
Direct (eco)toxicity in soil
The MPC_{soil} derivation for aniline is cited from the EU-RAR (EC, 2004a). Toxicity data of aniline to terrestrial organisms are shown in Table A6. 3 (acute) in Appendix 6.
The lowest EC50 value found for soil exposure of *Lactuca sativa* was 33 $mg.kg_{dw}^{-1}$ (Hulzebos *et al*., 1993 cited in EC, 2004a). In the EU-RAR for aniline (EC, 2004a), an assessment factor of 1000 was applied, resulting in a $PNEC_{soil}$ of 33 $\mu g.kg_{dw}^{-1}$ (24 $\mu g.kg_{ww}^{-1}$) in a soil containing 1.8% organic matter. However, the practicability of the test for risk assessment was questioned in the EU-RAR, because during the test the plants were initially exposed to free aniline, while later the plants were exposed to both free aniline in the pore water and bound aniline in the solid phase. Under natural conditions, soil organisms will mainly be exposed to the bound substance, as aniline is set free relatively slowly from agents and is always is equilibrium with the bound form.
In the EU-RAR for aniline, a $PNEC_{soil}$ of 11 $\mu g.kg_{ww}^{-1}$ is calculated from a $PNEC_{aqua}$ of 1.5 $\mu g.L^{-1}$, using EqP. However, the authors considered this approach not to be appropriate as only the exposure via pore water is considered by this model.
In the EU-RAR, toxicity of other aniline derivatives was investigated. This investigation showed that pre-incubation of soil with 3,4-dichloroaniline significantly reduced toxicity. However, on basis of the available information reduction of toxicity by pre-incubation of soil with aniline can not be estimated. Further testing with aniline was considered necessary to assess the effect of aniline in soil. The $PNEC_{soil}$ of 33 $\mu g.kg_{dw}^{-1}$ was used for risk assessment. Therefore, the $PNEC_{soil}$ of

33 $\mu g.kg_{dw}^{-1}$ is used to set the MPC_{soil}. Recalculation of the $PNEC_{soil}$ to standard soil gives $33 \times 10/1.8 = 183$ $\mu g.kg_{dw}^{-1}$ or 0.183 $mg.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of root crops is the most critical route. The $MPC_{human, soil}$ based on this route is 0.61 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the MPC_{soil} based on ecotoxicological data for soil organisms. Hence, MPC_{soil} is 0.18 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.6.2 SRC_{eco}

Two acute tests with *Lactuca sativa* are available with as test endpoint growth. Geometric mean of the two EC50 values is 270.8 $mg.kg_{dw}^{-1}$. An assessment factor of 10 has to be applied, resulting in an SRC_{eco} for soil of 27.1 $mg.kg_{dw}^{-1}$ Dutch standard soil.
Since only acute toxicity data for only one organism are available, the SRC_{eco} for soil also has to be calculated on basis of EqP departing from the SRC_{eco} for the water compartment. Using SRC_{eco} = 5.1 $mg.L^{-1}$ and log K_{oc} = 2.61 an SRC_{eco} based on EqP of 124 $mg.kg^{-1}$ standard soil is calculated. The lowest value is selected, therefore, the SRC_{eco} is 27.1 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.7 Epichlorohydrin

7.1.7.1 MPC

Direct ecotoxicity - equilibrium partitioning
No toxicity data of epichlorohydrin to terrestrial organisms are available. The MPC_{soil} is therefore calculated using EqP. To that end, the $MPC_{eco, water}$ of 0.65 $\mu g.L^{-1}$ and a log K_{oc} of 1.25 were used, together with the characteristics of Dutch standard soil. This results in an MPC_{soil} of 0.935 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of root crops is the most critical route. The $MPC_{human, soil}$ based on this route is 2.71 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the MPC_{soil} calculated using EqP, based on ecotoxicological data for the aquatic compartment. Hence, MPC_{soil} is 0.94 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.7.2 SRC_{eco}

The SRC_{eco} for soil is calculated on the basis of the SRC_{eco} for water using EqP. Using SRC_{eco} for water of 3.1 mg L^{-1} and log K_{oc} = 1.25, the SRC_{eco} for soil is calculated to be 4.48 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.8 1,2-Dibromoethane

7.1.8.1 MPC

Direct (eco)toxicity in soil and equilibrium partitioning
Acute toxicity data are available for bacteria, fungi and nematodes. However, since the percentage organic matter was not reported in the acute soil toxicity data, these data can not be recalculated to standard soil and will not be used for ERL derivation (see rejected data in Table A6. 12). The useful

toxicity data for terrestrial organisms are shown in Table A6. 8 (chronic) in Appendix 6. There is one chronic toxicity study available, that is useful for ERL derivation. Therefore, the MPC_{soil} has to be calculated both on the basis of this toxicity test and with EqP, departing from the $MPC_{eco, water}$. The NOEC from the one chronic soil toxicity study for germination of microsclerotia of *Verticillium dahliae* is 3.30 $mg.kg_{dw}^{-1}$. Using this value and an assessment factor of 1000, the MPC_{soil} is calculated as 3.30 $mg.kg_{dw}^{-1}$ /1000 = 3.3 $\mu g/kg_{dw}$ Dutch standard soil. Applying EqP to the $MPC_{eco, water}$ of 40 $ng.L^{-1}$ and a log K_{oc} of 1.80, the MPC_{soil} is 0.165 $\mu g.kg_{dw}^{-1}$. The lowest value is selected as MPC_{soil}, which is thus set at 0.165 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of root crops is the most critical route. The $MPC_{human, soil}$ based on this route is 0.0122 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the $MPC_{human, soil}$. Hence, MPC_{soil} is 0.0122 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.8.2 SRC_{eco}

The SRC_{eco} will be calculated both using the single available NOEC value in soil and on the basis of EqP using the $SRC_{eco, water}$. Using the NOEC of 3.30 $mg.kg_{dw}^{-1}$ and an assessment factor of 1 results in an SRC_{eco} of 3.30 $mg.kg_{dw}^{-1}$. Applying EqP to the $SRC_{eco, water}$ of 0.79 $mg.L^{-1}$ and using a log K_{oc} of 1.80 and a Henry coefficient of 63.7 $Pa.m^3.mol^{-1}$ gives an $SRC_{eco, soil}$ of 3.23 $mg.kg_{dw}^{-1}$. The $SRC_{eco, soil}$ values derived using both methods are more or less equal; the lowest of the two is selected. Hence, the $SRC_{eco, soil}$ is 3.23 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.9 Ethinylestradiol

7.1.9.1 MPC

Direct ecotoxicity - equilibrium partitioning
No ecotoxicity data could be found for terrestrial organisms. Therefore, the MPC_{soil} was derived by equilibrium partitioning. The overall log K_{oc} value of 3.34 as determined in section 2.9.3.1, is used for EqP calculations. Using a log K_{oc} of 3.34 and an MPC_{water} of 0.016 $ng.L^{-1}$, the resulting MPC_{soil} is 2.06 $ng.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning
The $MPC_{oral, min}$ derived in section 6.1.9.2 for secondary poisoning in the aquatic compartment is used for calculation of secondary poisoning in soil as well. The $MPC_{oral, min}$ is 13.3 $ng.kg_{fd}^{-1}$. $BCF_{earthworm}$ is calculated using the TGD QSAR and the selected log K_{ow} of 3.67, resulting in a value of 57 $L.kg_{wwt}^{-1}$. Further input for the calculation of $MPC_{soil, sp}$ are the selected values for log K_{oc} = 3.34 $L.kg^{-1}$ and $H = 8.04 \times 10^{-7}$ $Pa.m^3.mol^{-1}$. Using the equation presented in INS guidance (which is derived from TGD guidance), the calculated $MPC_{soil, sp}$ = 31.1 $ng.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of leafy crops is the most critical route. The $MPC_{human, soil}$ based on this route is 10.9 $ng.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the two derived MPC_{soil} values is selected, which is the MPC_{soil} based on equilibrium partitioning. Hence, MPC_{soil} is 2.06 $ng.kg_{dw}^{-1}$ Dutch standard soil.

7.1.9.2 SRC_{eco}

The SRC_{eco} for soil is calculated using EqP. Using a log K_{oc} of 3.34 and an $SRC_{eco, water}$ of 2.43 $ng.L^{-1}$, the resulting $SRC_{eco, soil}$ is 0.313 $\mu g.kg_{dw}^{-1}$ (Dutch standard soil).

Note. Since a complete overview of all relevant toxicity studies for birds and mammals was not made in this project, a geometric mean of all $MPC_{oral, min}$ values can not be derived. For this reason, an SRC_{eco} based on secondary poisoning has not been not derived.

7.1.10 Methyl bromide

7.1.10.1 MPC

Direct (eco)toxicity in soil

Collected toxicity data for terrestrial organisms are shown in Table A6. 4 (acute) in Appendix 6. Toxicity data are available for plants. The MPC_{soil} is calculated on the basis of the lowest determined effect concentration. The lowest EC50 value is an EC50 for germination of *Amaranthus retroflexus* of 2.5 $mg.kg_{dw}^{-1}$. Applying an assessment factor of 1000 results in an MPC_{soil} of 2.5 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.
Since more than one toxicity test result for soil organisms is available, the MPC_{soil} does not need to be determined using EqP. However, if EqP is applied to the $MPC_{eco, water}$ and using the geometric mean log K_{oc} of 0.606 and H = 685 $Pa.m^3.mol^{-1}$, the resulting $MPC_{soil, EqP}$ would be 2.4 $\mu g.kg_{dw}^{-1}$ standard soil, which is very close to the MPC_{soil} derived in the above section.

$MPC_{human, soil}$

Of the four human exposure routes considered, consumption of root crops is the most critical route. The $MPC_{human, soil}$ based on this route is 16.5 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}

The lowest of the two derived MPC_{soil} values is selected, which is the $MPC_{eco, soil}$, based on ecotoxicological data for soil organisms. Hence, MPC_{soil} is 2.5 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.10.2 SRC_{eco}

The SRC_{eco} is based on the geometric mean of the available EC50 values using an assessment factor of 10. This results in an SRC_{eco} of 0.727 $mg.kg_{dw}^{-1}$ standard soil. The SRC_{eco} is also calculated using EqP. To that end, the SRC_{eco} of 0.179 $\mu g.L^{-1}$, log K_{oc} of 0.606 and a Henry coefficient of 685 $Pa.m^3.mol^{-1}$ were used, together with the characteristics of Dutch standard soil. This results in an SRC_{eco} of 0.133 $\mu g.kg_{dw}^{-1}$ standard soil. The lowest value is selected, SRC_{eco} is 0.133 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

7.1.11 6PPD

7.1.11.1 MPC

Direct ecotoxicity - equilibrium partitioning

No ecotoxicity data could be found for terrestrial organisms. Therefore, the MPC_{soil} is derived by equilibrium partitioning. The $MPC_{eco, water}$ of 0.48 $\mu g.L^{-1}$, the selected log K_{oc} of 4.48 and a Henry coefficient of 9.39×10^{-2} $Pa.m^3.mol^{-1}$ were used, together with the characteristics of Dutch standard soil. This results in an MPC_{soil} of 0.853 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning
The NOAEL of 75 $mg.kg_{bw}^{-1}.d^{-1}$ reported in the OECD SIDS report (OECD, 2004) is used to calculated an $MPC_{oral, min}$. This NOAEL is based on feeding studies ranging from 13 weeks to 24 months exposure in both male and female rats. This NOAEL is converted to a NOEC of 750 $mg.kg_{fd}^{-1}$ using a conversion factor of 10 $g_{bw}.g_{fd}^{-1}.d^{-1}$. Since the study is chronic, an assessment factor of 30 is applied to calculate the $MPC_{oral, min}$, which is 25 $mg.kg_{fd}^{-1}$.
$BCF_{earthworm}$ is calculated using the TGD QSAR and the selected log K_{ow} of 5.41, resulting in a value of 3085 $L.kg_{wwt}^{-1}$. Further input for the calculation of $MPC_{soil, sp}$ are the selected values for log K_{oc} = 4.48 $L.kg^{-1}$ and $H = 9.39\times10^{-2}$ $Pa.m^3.mol^{-1}$. Using the equation presented in INS guidance (which is derived from TGD guidance), the calculated $MPC_{soil, sp}$ = 15.7 $mg.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of leafy crops is the most critical route. The $MPC_{human, soil}$ based on this route is 2.4 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Selection of MPC_{soil}
The lowest of the three derived MPC_{soil} values is selected, which is the MPC_{soil} based on equilibrium partitioning. Hence, MPC_{soil} is 0.853 $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.11.2 SRC_{eco}
The SRC_{eco} is also calculated using equilibrium partitioning. The $SRC_{eco, water}$ of 0.021 $mg.L^{-1}$ and the same parameters as mentioned in the above section on MPC_{soil} (section 7.1.11.1) are used as input. This results in an $SRC_{eco, soil}$ of 37.3 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Note. Since a complete overview of all relevant toxicity studies for birds and mammals was not made in this project, a geometric mean of all $MPC_{oral, min}$ values can not be derived. For this reason, an SRC_{eco} based on secondary poisoning has not been not derived.

7.1.12 3,3'-Dichlorobenzidine

7.1.12.1 MPC
Direct toxicity/equilibrium partitioning
No ecotoxicity data could be found for terrestrial organisms. Therefore, the MPC_{soil} is derived by equilibrium partitioning. The $MPC_{eco, water}$ of 0.058 $\mu g.L^{-1}$, the selected log K_{oc} of 3.99 and a Henry coefficient of 1.45×10^{-3} $Pa.m^3.mol^{-1}$ were used, together with the characteristics of Dutch standard soil. This results in an MPC_{soil} of 33.4 $\mu g.kg_{dw}^{-1}$ Dutch standard soil.

Secondary poisoning
The $MPC_{oral, min}$ derived in section 6.1.12.2 for secondary poisoning in the aquatic compartment is used for calculation of secondary poisoning in soil as well. The $MPC_{oral, min}$ is 1.33 $mg.kg_{fd}^{-1}$.
$BCF_{earthworm}$ is calculated using the TGD QSAR and the selected log K_{ow} of 3.51, resulting in a value of 40 $L.kg_{wwt}^{-1}$. Further input for the calculation of $MPC_{soil, sp}$ are the selected values for log K_{oc} = 3.99 $L.kg^{-1}$ and $H = 1.45\times10^{-3}$ $Pa.m^3.mol^{-1}$. Using the equation presented in INS guidance (which is derived from TGD guidance), the calculated $MPC_{soil, sp}$ = 14.4 $mg.kg_{dw}^{-1}$ Dutch standard soil.

$MPC_{human, soil}$
Of the four human exposure routes considered, consumption of leafy crops is the most critical route. The $MPC_{human, soil}$ based on this route is 2.94×10^{-6} $mg.kg_{dw}^{-1}$ Dutch standard soil.

The $MPC_{human, soil}$ is much lower than the $MPC_{eco, soil}$ and the $MPC_{sp, soil}$, which is caused by the carcinogenicity of DCB. The human toxicological risk limit on which the $MPC_{human, soil}$ is based, is derived using a rather low NRL (negligible risk level). Since the NRL was not based on a NOAEL (see section 4.12.3), it could not be used for derivation of an MPC for secondary poisoning. Moreover, the NRL is expressed as a 10^{-6} probability after life time exposure (70 years), which is considered an inappropriate endpoint for secondary poisoning in the terrestrial environment. Therefore, a literature search was performed to retrieve NOAEL data for birds and/or mammals, on which the derivation of $MPC_{sp, soil}$ was based (see section 4.12.4).

Selection of MPC_{soil}
The lowest of the three derived MPC_{soil} values is selected, which is the MPC_{soil} based on EqP. Hence, MPC_{soil} is 2.94×10^{-6} $mg.kg_{dw}^{-1}$ Dutch standard soil.

7.1.12.2 SRC_{eco}
The SRC_{eco} is also calculated using equilibrium partitioning. The $SRC_{eco, water}$ of 0.096 $mg.L^{-1}$ and the same parameters as mentioned in the above section on MPC_{soil} (section 7.1.12.1) are used as input. This results in an $SRC_{eco, soil}$ of 55.3 $mg.kg_{dw}^{-1}$ Dutch standard soil.

Note. Since no toxicity studies for birds and mammals were retrieved (see section 4.12.4) , a geometric mean of all $MPC_{oral, min}$ values can not be derived. For this reason, an SRC_{eco} based on secondary poisoning has not been not derived.

7.2 ERL derivation for sediment

7.2.1 PentaBDE

7.2.1.1 MPC
Freshwater
The $MPC_{eco, sediment}$ derivation for pentaBDE is cited from the EU-RAR (EC, 2001). Sediment toxicity data for pentaBDE are presented in Table A7. 1 (chronic) in Appendix 7. Data selected for ERL derivation are shown in Table A3. 1.
For pentaBDE, three 28 day toxicity tests with sediment-dwelling organisms are available, *viz*. *Lumbriculus variegatus*, *Hyalella azteca* and *Chironomus riparius*. These organisms represent different living and feeding conditions. In the EU-RAR for pentaBDE, an assessment factor of 10 is applied to the lowest of the available NOECs. The lowest NOEC available is 3.1 $mg.kg_{dw}^{-1}$ for *Lumbriculus variegatus*, which is equivalent to 15.5 $mg.kg_{dw}^{-1}$ standard EU sediment. Note that in the EU-RAR (EC, 2001) this recalculation to standard (EU) sediment was performed using f_{oc} = 0.05, for bulk sediment from the TGD and an assumed organic carbon content of 1% in the test. The latter value was an assumption, since the reported value for organic *matter* content in the *L. variegatus* test was <2% (EC, 2001).
For the Dutch ERL derivation, the NOEC is converted to Dutch standard sediment (containing 5.88% organic carbon). Thus, a NOEC of 3.1 $mg.kg_{dw}^{-1}$ standard EU sediment yields a NOEC of 18.3 $mg.kg_{dw}^{-1}$ Dutch standard sediment. Applying the assessment factor of 10 results in an $MPC_{eco, sediment}$ of 1.83 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

Marine
In order to derive a $PNEC_{sediment, marine}$, an assessment factor of 50 should is applied to the NOEC of 18.3 $mg.kg_{dw}^{-1}$ (expressed in Dutch standard sediment), since data for three different species are available, but no data for saltwater species are available. The resulting $MPC_{eco, marine sediment}$ is thus 18.3/50 = 0.37 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.1.2 SRC_{eco}

Freshwater
The $SRC_{eco, sediment}$ is calculated as the geometric mean of three available NOEC values expressed in Dutch standard sediment (Table A3. 1): 18.2, 37.0 and 94.1 $mg.kg_{dw}^{-1}$, resulting in an $SRC_{eco, sediment}$ of 40 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

Marine
The SRC_{eco} for marine sediment, $SRC_{eco, marine sediment}$, is set equal to the $SRC_{eco, sediment}$ (SRC_{eco} for freshwater sediment): $SRC_{eco, marine sediment}$ = 40 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.2 p-*tert*-octylphenol

7.2.2.1 MPC

Freshwater
The report by the UK environment agency (Brooke *et al.*, 2005), which is the basis for this ERL derivation, states that no data on toxicity of p-*tert*-octylphenol to sediment organisms were available. The $MPC_{eco, sediment}$ is therefore calculated using EqP. To that end, the $MPC_{eco, water}$ of 0.122 $\mu g.L^{-1}$ and the log K_{oc} of 3.43 were used, together with the characteristics of Dutch standard sediment. This results in an $MPC_{eco, sediment}$ of 19.6 $\mu g.kg_{dw}^{-1}$ Dutch standard sediment.

Marine
The $MPC_{eco, marine sediment}$ is calculated using EqP and the $MPC_{eco, marine}$. This results in an $MPC_{eco, marine sediment}$ of 1.96 $\mu g.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.2.2 SRC_{eco}

Freshwater
The $SRC_{eco, sediment}$ is calculated using EqP on the basis of the $SRC_{eco, water}$. The following values were used: $SRC_{eco, water}$ = 40.8 $\mu g.L^{-1}$ and log K_{oc} = 3.43 based on chronic toxicity data. The $SRC_{eco, sediment}$ is calculated to be 6.54 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

Marine
The SRC_{eco} for marine sediment, $SRC_{eco, marine sediment}$, is set equal to the $SRC_{eco, sediment}$ (SRC_{eco} for freshwater sediment): $SRC_{eco, marine sediment}$ = 6.54 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.3 Benzo[*b*]fluoranthene

7.2.3.1 MPC

Freshwater
The $MPC_{eco, sediment}$ derivation for benzo[*b*]fluoranthene is cited from the draft EU-RAR on coal tar pitch (EC, 2006b). Toxicity data are presented in Table A7. 2 in Appendix 7.

Citation from draft EU-RAR on PCTHT (EC, 2006b):
'The only benthic species that was tested was the marine crustacean *Rhepoxynius abronius* (Boese *et al*., 1998, cited in EC, 2006b). Up to concentrations of 180 $mg.kg_{dw}^{-1}$, recalculated to a sediment with 10% organic carbon, no effects were observed. The PNEC for sediment has to be derived by equilibrium partitioning (…).'

Since no effect concentration was established, this toxicity result that can not be used to derive an MPC, hence toxicity data for benthic organisms are not available for benzo[*b*]fluoranthene. Since a read across was performed with benzo[*k*]fluoranthene for the derivation of the $MPC_{eco, water}$, toxicity data for benthic organisms for benzo[*k*]fluoranthene have been taken into consideration as well. Toxicity data are presented in Table A7. 3 in Appendix 7.

Citation from draft EU-RAR on PCTHT (EC, 2006b):
'Benzo[*k*]fluoranthene in freshwater sediment was tested with three species. For *Hyalella azteca* and larvae of *Chironomus riparius*, no toxicity was observed up to a concentration of 300 $mg.kg_{dw}^{-1}$, recalculated to a sediment with 10% organic carbon. At this concentration 45% effect was reached in a 48-h toxicity test with *Daphnia magna* (Verrhiest *et al*., 2001, cited in EC, 2006b). However, *Daphnia magna* is rather an aquatic organism than a benthic organism. With a sediment concentration of 1500 $mg.kg_{dw}^{-1}$, recalculated to sediment with 10% organic carbon, the overlying water is probably saturated. Therefore, this value should be considered as 45% mortality at the aqueous solubility.'

'Because no toxicity data can be used for deriving the PNEC, the PNEC for sediment must be calculated by equilibrium partitioning, resulting in a value of 1.38 $mg{\cdot}kg_{dw}^{-1}$ for the fresh water environment (…)'.

The $PNEC_{sediment}$ is equal to an $MPC_{eco, sediment}$ of 0.81 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

Marine
The PNEC for marine sediment was also derived by equilibrium partitioning, resulting in a value of 0.14 $mg.kg_{dw}^{-1}$ for the marine environment. This is equal to an $MPC_{eco, marine\ sediment}$ of 0.081 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.3.2 SRC_{eco}

Freshwater
The $SRC_{eco, sediment}$ is calculated using EqP, based on the $SRC_{eco, water}$. The following values were used: $SRC_{eco, water} = 0.17\ \mu g.L^{-1}$, log K_{oc} = 5.91 and $H = 0.051\ Pa.m^3.mol^{-1}$. The resulting $SRC_{eco, sediment}$ is 8.3 $mg.kg_{dw}^{-1}$ Dutch standard sediment.
Marine
The SRC_{eco} for marine sediment, $SRC_{eco, marine\ sediment}$, is set equal to the $SRC_{eco, sediment}$ (SRC_{eco} for freshwater sediment): $SRC_{eco, marine\ sediment}$ = 8.3 $mg.kg_{dw}^{-1}$ Dutch standard sediment.

7.2.4 6PPD

Freshwater

7.2.4.1 MPC

In the absence of toxicity data of 6PPD for sediment dwelling organisms, the $MPC_{eco, sediment}$ is calculated using EqP. To that end, the $MPC_{eco, water}$ of 0.48 $\mu g.L^{-1}$, the Henry coefficient of

9.39×10^{-2} Pa.m^3.mol^{-1} and the log K_{oc} of 4.48 were used, together with the characteristics of Dutch standard sediment. This results in an $MPC_{eco,\ sediment}$ of 0.854 mg.kg$_{dw}^{-1}$ Dutch standard sediment.

Marine
The $MPC_{eco,\ marine\ sediment}$ is calculated using EqP and the $MPC_{eco,\ marine}$. This results in an $MPC_{eco,\ marine\ sediment}$ of 0.0854 mg.kg$_{dw}^{-1}$ or 85.4 µg.kg$_{dw}^{-1}$ Dutch standard sediment.

7.2.4.2 SRC_{eco}

Freshwater
The $SRC_{eco,\ sediment}$ for 6PPD is calculated using EqP. Using the $SRC_{eco,\ water}$ of 0.021 mg.L^{-1}, the Henry coefficient of 9.39×10^{-2} Pa.m^3.mol^{-1} and the log K_{oc} of 4.48, the $SRC_{eco,\ sediment}$ is calculated to be 37.3 mg.kg$_{dw}^{-1}$ Dutch standard sediment.

Marine
The SRC_{eco} for marine sediment, $SRC_{eco,\ marine\ sediment}$, is set equal to the $SRC_{eco,\ sediment}$ (SRC_{eco} for freshwater sediment): $SRC_{eco,\ marine\ sediment}$ = 37.3 mg.kg$_{dw}^{-1}$ Dutch standard sediment.

7.2.5 3,3'-Dichlorobenzidine

7.2.5.1 MPC

Freshwater
In the absence of toxicity data of DCB for sediment dwelling organisms, the $MPC_{eco,\ sediment}$ is calculated using EqP. To that end, the $MPC_{eco,\ water}$ of 0.058 µg.L^{-1}, the Henry coefficient of 1.45×10^{-3} Pa.m^3.mol^{-1} and the log K_{oc} of 3.99 were used, together with the characteristics of Dutch standard sediment. This results in an $MPC_{eco,\ sediment}$ of 33.5 µg.kg$_{dw}^{-1}$ Dutch standard sediment.

Marine
The $MPC_{eco,\ marine\ sediment}$ is calculated using EqP and the $MPC_{eco,\ marine}$. This results in an $MPC_{eco,\ marine\ sediment}$ of 0.00335 mg.kg$_{dw}^{-1}$ or 3.35 µg.kg$_{dw}^{-1}$ Dutch standard sediment.

7.2.5.2 SRC_{eco}

Freshwater
The $SRC_{eco,\ sediment}$ for DCB is calculated using EqP. Using the $SRC_{eco,\ water}$ of 0.096 mg.L^{-1}, the Henry coefficient of 1.45×10^{-3} Pa.m^3.mol^{-1} and the log K_{oc} of 3.99, the $SRC_{eco,\ sediment}$ is calculated to be 55.5 mg.kg$_{dw}^{-1}$ Dutch standard sediment.

Marine
The SRC_{eco} for marine sediment, $SRC_{eco,\ marine\ sediment}$, is set equal to the $SRC_{eco,\ sediment}$ (SRC_{eco} for freshwater sediment): $SRC_{eco,\ marine\ sediment}$ = 55.5 mg.kg$_{dw}^{-1}$ Dutch standard sediment.

7.2.6 Remaining compounds

No toxicity data or physicochemical data have been collected for isodrin. For this reason, an MPC or SRC_{eco} for sediment is not derived. For DNOC, aniline, epichlorohydrin, 1,2-dibromoethane, ethinylestradiol and methyl bromide, $MPC_{eco,\ sediment}$ and $SRC_{eco,\ sediment}$ are not derived, since log $K_{p,\ susp\text{-}water}$ is < 3 for these compounds.

7.3 ERL derivation for groundwater

Table 56 shows the two MPC values that have been derived for the groundwater compartment for each of the twelve substances investigated. The methodology to derive the two values is described in INS guidance in detail (Van Vlaardingen and Verbruggen, 2007). In short: the $MPC_{eco, gw}$ is equal to the $MPC_{eco, water}$ and the $MPC_{human, gw}$ is set equal to the $MPC_{dw, water}$.

Table 56. $MPC_{eco, gw}$ and $MPC_{human, gw}$ for twelve substances.

Compound	$MPC_{eco, gw}$ [µg.L^{-1}]	$MPC_{human, gw}$ [µg.L^{-1}]	MPC_{gw} [µg.L^{-1}]
pentaBDE	0.53	0.00091	0.00091
p-*tert*-octylphenol	0.122	525	0.12
benzo[*b*]fluoranthene	0.017	0.18	0.017
DNOC	9.2	1	1
aniline	1.5	5.0	1.5
epichlorohydrin	0.65	0.10	0.10
1,2-dibromoethane	0.040	0.0018	0.0018
ethinylestradiol	0.000016	0.0035	0.000016
methyl bromide	3.2	4.9	3.2
6PPD	0.48	2625	0.48
3,3'-dichlorobenzidine	0.058	0.00015	0.00015

7.4 ERL derivation for air

Human toxicological risk limits for inhalation exposure were searched for all twelve compounds. Risk limits were retrieved for five compounds: aniline, epichlorohydrin, 1,2-dibromoethane, methyl bromide and 3,3'-dichlorobenzidine (see the following sections for the sources of these risk limits). Ecotoxicological data for exposure via air are available for three compounds: aniline, 1,2-dibromoethane and methyl bromide. However, the EU-TGD does not provide guidance for deriving a $PNEC_{air}$. Therefore, the $MPC_{eco, air}$ is derived in analogy with other compartments (as was done in De Jong *et al.*, 2007). However, since guidance on ERL derivation for exposure via air has not been worked out definitively, we propose to designate all MPC_{air} values as 'preliminary'.

7.4.1 Aniline

Ecotoxicity

Few ecotoxicological data for exposure via air were presented in the EU-RAR (EC, 2004a). The data are presented in Table A8. 1. A $PNEC_{plant}$ was derived on the basis of the NOEC of 0.0003 mg.L^{-1} or 0.3 mg.m^{-3} found for *Brassica pekinensis*. In the EU-RAR, an assessment factor of 50 was used to derive the $PNEC_{plant}$ since the exposure duration in the test was not considered to be representative of chronic exposure. $PNEC_{plant} = MPC_{eco, air}$ = 0.3 mg.m^{-3} / 50 = of 6 µg.m^{-3}.

Human toxicological risk limit

US EPA has derived an RfC of 1 µg.m^{-3} (1993; US EPA, 2007b). Although the US EPA classifies aniline as a probable human carcinogen (B2), an inhalation risk limit based on carcinogenicity was not be derived, probably due to a lack of reliable data. The RfC is thus based on non-carcinogenic toxic effects.

Selection of MPC_{air}
The lowest of the two available MPC values is selected as the environmental risk limit MPC_{air}. The $MPC_{human, air}$ is the lowest value. Therefore, the preliminary MPC_{air} for aniline is 1 $\mu g.m^{-3}$.

7.4.2 Epichlorohydrin

Ecotoxicity
No ecotoxicological data for exposure via air were found. Hence, an $MPC_{eco, air}$ could not be derived.

Human toxicological risk limit
US EPA has derived a risk specific dose for carcinogenic risk from inhalation exposure of 0.8 $\mu g.m^{-3}$ at a risk level of 10^{-6} for lifetime exposure (1994; US EPA, 2007b). The US EPA classifies epichlorohydrin as a probable human carcinogen (B2).

Selection of MPC_{air}
Ecotoxicological data using exposure via air are lacking. Therefore, the preliminary MPC_{air} is set equal to the $MPC_{human, air}$. Therefore, the preliminary MPC_{air} for epichlorohydrin is 0.8 $\mu g.m^{-3}$.

7.4.3 1,2-Dibromoethane

7.4.3.1 MPC

Ecotoxicity
The toxicity data for organisms exposed to 1,2-dibromethane via air are shown in Table A8. 1 (acute) and Table A8. 4 (chronic) in Appendix 8. Data selected for ERL derivation are shown in Table A4. 1 in Appendix 4. The MPC_{air} is calculated on the basis of the lowest determined effect concentration. The lowest L(E)C50 value found was an LC50 of 0.243 $mg.L^{-1}$ for eggs of *Callosobruchus chinensis*. Applying an assessment factor of 1000 results in an $MPC_{eco, air}$ of 0.243 $\mu g.L^{-1}$, which is equal to 0.243 $mg.m^{-3}$.

Human toxicological risk limit
A tolerable concentration in air (TCA) has not been derived for 1,2-dibromoethane. US EPA has derived a risk specific dose for carcinogenic risk from inhalation exposure of 2×10^{-3} $\mu g.m^{-3}$ at a risk level of 10^{-6} for lifetime exposure (2004; US EPA, 2007b). It is proposed to set the $MPC_{human, air}$ equal to the risk level derived by the US EPA.

Selection of MPC_{air}
The lowest of the two available MPC values is selected as the environmental risk limit MPC_{air}. The $MPC_{human, air}$ is the lowest value. Therefore, the preliminary MPC_{air} for 1,2-dibromoethane is 2×10^{-3} $\mu g.m^{-3}$.

7.4.4 Methyl bromide

7.4.4.1 MPC

Ecotoxicity
The toxicity data for organisms exposed to methyl bromide via air are shown in Table A8. 3. Data selected for ERL derivation are shown in Table A4. 2 in Appendix 4. The MPC_{air} is calculated on the basis of the lowest determined effect concentration. The lowest L(E)C50 value found was an LC50 of 0.851 $mg.L^{-1}$ for eggs of *Callosobruchus chinensis*. Applying an assessment factor of 1000 results in an MPC_{air} of 0.851 $\mu g.L^{-1}$, which is equal to 0.851 $mg.m^{-3}$.

Human toxicological risk limit
A tolerable concentration in air (TCA) of 0.1 $mg.m^{-3}$ has been derived by RIVM (Van der Heijden *et al.*, 1987). The TCA is taken as $MPC_{human, air}$.

Selection of MPC_{air}
The lowest of the two available MPC values is selected as the environmental risk limit MPC_{air}. The $MPC_{human, air}$ is the lowest value. Therefore, the preliminary MPC_{air} for methyl bromide is 0.1 $mg.m^{-3}$ or 100 $\mu g.m^{-3}$.

7.4.5 3,3'-Dichlorobenzidine (DCB)

Ecotoxicity
No ecotoxicological data for exposure via air were found. Hence, an $MPC_{eco, air}$ could not be derived.

Human toxicological risk limit
US EPA has derived a risk specific dose for carcinogenic risk from inhalation exposure for benzidine of 2.0×10^{-5} $\mu g.m^{-3}$ at a risk level of 10^{-6} for lifetime exposure (1993; US EPA, 2007b). Using a factor of 10 to account for the lower carcinogenic potency of DCB in relation to benzidine (see section 4.12.3), a risk specific dose of 2.0×10^{-4} $\mu g.m^{-3}$ is derived for DCB. Hence, the $MPC_{human, air}$ is of 2.0×10^{-4} $\mu g.m^{-3}$.

Selection of MPC_{air}
Ecotoxicological data using exposure via air are lacking. Therefore, the preliminary MPC_{air} is set equal to the $MPC_{human, air}$. The preliminary MPC_{air} for DCB is 2.0×10^{-4} $\mu g.m^{-3}$.

8. Overview and comparison of ERLs

8.1 Final MPCs derived in this report

Table 58 shows all selected, final MPC values. Values presented in the table with a shaded background (and followed by the letter H) are MPCs derived as $MPC_{human, comp}$, i.e. these values are based on a human toxicological risk limit. The values presented without shading were derived using ecotoxicological data (and are followed by the letter E), on the basis of WFD and/or TGD guidance as described in Chapters 6 and 7.

8.2 Comparison of MPCs and *ad hoc*-MPCs

A comparison between the existing *ad hoc*-MPCs and the MPCs derived in this report is shown in Table 57. See Table 43 for background information on the various *ad hoc*-MPC values. The column 'Critical route' behind the MPC_{water} column, shows which route of MPC derivation has led to the final MPC_{water}. Abbreviations are explained in the footnotes to the table. MPCs shown in **bold** are lower than both existing *ad hoc*-MPC(s).

Table 57. Comparison between ad hoc-MPC values and MPC values derived in this report.

Compound	MPC_{water} This report [$\mu g.L^{-1}$]	Critical route	*ad hoc* MPC_{water} RIZA [$\mu g.L^{-1}$]	*ad hoc* MPC_{water} RIVM [$\mu g.L^{-1}$]	MPC_{soil} This report [$\mu g.kg_{dw}^{-1}$]	Critical Route[f]	*ad hoc* MPC_{soil} RIVM [$\mu g.kg_{dw}^{-1}$]
pentaBDE	**2.9×10^{-8}**	H,F	0.014	0.53	4.3×10^{-4}	H,M	
p-*tert*-octylphenol	0.12	E,Di	0.122; 3.2	0.00423	19	E, EqP	1
benzo[*b*]fluoranthene	**0.017**[d]	E,Di	0.025	0.024	0.40	H,L	
isodrin	0.01[a]		0.008	8.2×10^{-4}			4.29
DNOC	**0.1**	H,Dw	196; 21[b]	–[e]	170	E,Di	
aniline	1.5	E,Di	0.08	0.42	183	E,Di	
epichlorohydrin	**0.10**	H,Dw	12	2.95	0.94	E, EqP	0.43
1,2-dibromoethane	0.0018	H,Dw	4.8	5.96×10^{-5}	0.012	H,R	1.98×10^{-5}
ethinylestradiol	**1.6×10^{-5}**	E,Di	1	0.189	**0.0021**	E, EqP	7.3
methyl bromide	3.2	E,Di	7000[c]; 7[c]	0.42	2.5	E,Di	0.059
6PPD	0.48	E,Di	2.4	0.0538	863	E, EqP	0.39
3,3'-dichlorobenzidine	**5.2×10^{-6}**	H,F	1	2.56×10^{-4}	0.0029	H,L	3.92×10^{-4}

Notes
All values calculated in this report are displayed in two significant digits. Values lower than 1 $ng.L^{-1}$ (0.001 $\mu g.L^{-1}$) are displayed in scientific notation.
[a]Standard set in 88/347/EEC (EC, 1988; daughter directive of 76/464/EC; EC, 1976) four the sum of four drins.
[b]RIZA has derived two *ad hoc*-MPC values for DNOC: one tabulated as 2-methyl-4,6-dinitrophenol, the other tabulated as DNOC.
[c]RIZA has derived two *ad hoc*-MPC values for methyl bromide.
[d]Preliminary MC value.
[e]RIVM has not derived an *ad hoc*-MPC for DNOC.
[f]Abbreviations used in column 'Critical route':
E = based on ecotoxicological data.
E,Di = based on direct toxicity (ecotoxicological data).
E,EqP = based on equilibrium partitioning.
H = based on human toxicological risk limit.
H,Dw = based on drinking-water consumption.
H,F = based on human fish consumption.
H,L = based on consumption of leaf crops.
H,M = based on consumption of meat.

Table 58. Overview of all MPC values derived in this report, derivation route and assessment factor (where appropriate).

Compartment⇨	Freshwater			Marine water			Sediment			Soil			Groundwater		Air		
Compound⇩	MPC_{water} [µg.L^{-1}]	Critical route	AF	MPC_{marine} [µg.L^{-1}]	Critical route	AF	$MPC_{sediment}$ [µg.kg$_{dw}^{-1}$]	Critical route	AF	MPC_{soil} [µg.kg$_{dw}^{-1}$]	Critical route	AF	MPC_{gw} [µg.L^{-1}]	Critical route	MPC_{air} [µg.m^{-3}]	Critical route	AF
PentaBDE	2.9×10^{-8}	H,F		2.9×10^{-8}	H,F		1800	E,Di	10	4.3×10^{-4}	H,M		9.1×10^{-4}	H,Dw			
OP	0.12	E,Di	50	0.012	E, Di	100	20	E, EqP		19	E,EqP		0.12	E,Di			
benzo[b]fluoranthene	0.017[a]	E,Di	10	0.0017[a]	E		810	E, EqP		0.40[d]	H,L		0.017	E,Di			
isodrin	0.010[b]			0.0050[b]													
DNOC	0.1	H,Dw		n.d.						170	E,Di	100	1	H,Dw			
Aniline	1.5	E,Di	10	0.15	E, Di	100				180	E,Di	1000	1.5	E,Di	1[a]	H	
Epichlorohydrin	0.10[d]	H,Dw		0.065	E, Di	100				0.94	E,EqP		0.10[d]	H,Dw	0.8[a,c,d]	H	
1,2-dibromoethane	0.0018[d]	H,Dw		0.0033[d]	H,F					0.012[d]	H,R		0.0018[d]	H,Dw	0.0020[a,d]	H	
ethinylestradiol	1.6×10^{-5}	E,Di	10	1.6×10^{-6}	E, Di	100				0.0021	E,EqP		1.6×10^{-5}	E,Di			
methyl bromide	3.2	E,Di	100	0.32	E, Di	1000				2.5	E,Di	1000	3.2	E,Di	100[a]	H	
6PPD	0.48	E,Di	50	0.048	E, Di	500	850	E, EqP		860	E,EqP		0.48	E,Di			
DCB	5.2×10^{-6} [d]	H,F		5.2×10^{-9} [d]	H,F		33	E, EqP		0.0029[d]	H,L		1.5×10^{-4} [d]	H,Dw	2.0×10^{-4}[a,c,d]	H	1000

Notes and explanation of symbols

All values calculated in this report are displayed in two significant digits. Values originating from other sources may be displayed in 1 significant digit; e.g. a fixed standard like the MPC_{water} for DNOC, which is a DW standard from CD 98/83/EC (EC, 1998).

Values lower than 0.001 µg.L^{-1} are displayed in scientific notation.

MPC values derived based on human toxicological risk limits are shown shaded.

MPC values in sediment and soil are expressed in mg.kg^{-1} dry weight Dutch standard soil.

[a]Preliminary MPC value.

[b]Standard set in 88/347/EEC (EC, 1988; daughter directive of 76/464/EC; EC, 1976) four the sum of four drins.

[c]Ecotoxicological data for exposure via air were not found.

[d]This standard is derived from a human toxicological risk limit based on a cancer risk of 1:10^{-6} after life-long exposure.

n.d. = not determined.

AF = assessment factor.

E = based on ecotoxicological data.

- E,Di = based on direct toxicity (ecotoxicological data).
- E,EqP = based on equilibrium partitioning.

H = based on human toxicological risk limit.

- H,Dw = based on drinking-water consumption.
- H,F = based on human fish consumption.
- H,L = based on consumption of leaf crops.
- H,M = based on consumption of meat.
- R = based on consumption of root crops.

8.3 Comparison of MPCs and MAC_{eco}s

The MAC_{eco} (maximum acceptable concentration for the ecosystem) is an ERL that is new to the Dutch framework of standard setting. The MAC_{eco} is an environmental quality standard that should protect aquatic ecosystems against possible acute, transient exposure peaks. The MAC_{eco} should not be exceeded at any time.

MAC lower than MPC
In some cases, the MAC_{eco} may be lower than the MPC. This can be caused by the use of different assessment factors for derivation of the two ERLs and it is also more likely to occur for those compounds that have a lowest acute toxicity test result (LC50 or EC50) which is close to the lowest chronic value (NOEC or EC10) in the toxicity data set. This is the case for p-*tert*-octylphenol, where the MPC is from a NOEC of 6.1 $\mu g.L^{-1}$ (AF = 50) and the MAC_{eco} is derived from an LC50 of 13.3 $\mu g.L^{-1}$ (AF=100). There is also the possibility that the MPC is set equal to the $MPC_{hh\ food,\ water}$ or the $MPC_{dw,\ water}$. The maximum difference for the twelve compounds investigated here is less than a factor of 2.
MAC_{eco} values below the MPC are not deemed realistic, since this would imply that one expects acute toxic effects at concentrations below the ERL that protects for chronic exposure. Therefore, in those cases where the MAC_{eco} was lower than the MPC, the MAC_{eco} was set equal to the MPC.

Table 59. Comparison between final MPC_{water} values and MAC_{eco} values.

Compound	Derived MAC_{eco} [$\mu g.L^{-1}$]	MPC_{water} [$\mu g.L^{-1}$]	Ratio MAC_{eco}/MPC	MAC_{eco} proposal [$\mu g.L^{-1}$]
pentaBDE	n.p.[a]	2.9×10^{-8}		n.p.
p-*tert*-octylphenol	0.13	0.12	1.1	0.12
benzo[*b*]fluoranthene	n.p.[a]	0.017[c]		n.p.
isodrin	n.d.[b]	0.010		n.d.
DNOC	0.66	0.1	6.6	0.66
aniline	1.0	1.5	0.68	1.5
epichlorohydrin	6.5	0.10	62	6.5
1,2-dibromoethane	0.40	0.0018	229	0.40
ethinylestradiol	0.56	1.6×10^{-5}	35000	0.56
methyl bromide	7.0	3.2	2.2	7.0
6PPD	0.28	0.48	0.58	0.48
3,3'-dichlorobenzidine	0.058	5.2×10^{-6}	11139	0.058

n.d. = not derived.
n.p. = not possible to derive a standard.
[a]lack of acute toxicity data (incomplete base set).
[b]no toxicity data were searched since a fixed standard was available.
[c]Preliminary MPC value.

9. Discussion and final ERLs

9.1 Influence of WFD guidance on ERL derivation

The incorporation of WFD guidance into the methodology of environmental risk limit derivation (into INS framework in the Netherlands) and a comparable methodology for the compartments soil, groundwater and air (introduced at the Dutch national level only) results in ERLs that cover both the human and ecotoxicological protection objectives.
Of the twelve compounds treated in this report, we derived ERLs for eleven compounds, since for isodrin, only the legally binding Σ drins standard for surface water was reported. For six of the compounds, the MPC_{water} was determined by ecotoxicological data and for five compounds, a human toxicological risk limit determined the MPC_{water}. Typically, for compounds that are toxic to humans and have potential to bioaccumulate, human consumption of fish and sea fruit is the route determining the MPC (e.g. pentaBDE, 3,3'-dichlorobenzidine). For compounds that are toxic to humans or (suspect) carcinogenic, but less bioaccumulative, the drinking-water route often prevails (e.g. epichlorohydrin, 1,2-dibromoethane). For compounds that are less toxic to humans, direct effects on aquatic species often determine the MPC_{water} rather than indirect exposure of humans. In this report, these compounds are: p-*tert*-octylphenol, aniline, ethinylestradiol, methyl bromide, 6PPD and benzo[*b*]fluoranthene. The latter compound should be treated with care, since it is potentially carcinogenic (R45), but an MPC via fish consumption could not be derived due to lack of a BCF and an MPC_{oral}.
In marine water, the same division of critical routes determining the MPC is found as for freshwater, with the exception of the drinking-water route. Drinking water is assumed not to be prepared from sea water within WFD guidance.
ERLs for sediment are always determined by ecotoxicological data since there are no indirect exposure scenarios for humans exposed to sediment. With the introduction of WFD guidance, ERLs for sediment are only derived when the partitioning coefficient suspended matter-water is > 1000 ($\log K_{p,\ susp\text{-}water} > 3$). Due to a general lack of sediment ecotoxicity data, ERLs for sediment are often based on equilibrium partitioning (EqP), as is the case here for four of the five compounds for which an $MPC_{sediment}$ was derived: EqP for p-*tert*-octylphenol, benzo[*b*]fluoranthene, 6PPD and 3,3'-dichlorobenzidine and direct toxicity for pentaBDE.
For soil, four out of eleven ERLs were derived based on indirect exposure of humans (pentaBDE, benzo[*b*]fluoranthene, 1,2-dibromoethane, and 3,3'-dichlorobenzidine). For the remaining seven compounds, ecotoxicological data determined the ERL: soil ecotoxicological data were available for DNOC, aniline and methyl bromide, while aquatic toxicity data and EqP were used for p-*tert*-octylphenol, epichlorohydrin, ethinylestradiol and 6PPD.
For groundwater, the lowest of the MPC protecting aquatic ecosystems ($MPC_{eco,\ water}$) or drinking-water ($MPC_{dw,\ water}$) is selected in order to protect both objectives. The MPC based on drinking-water has determined the MPC for five compounds: benzo[*b*]fluoranthene, aniline, epichlorohydrin, 1,2-dibromoethane, and 3,3'-dichlorobenzidine.

9.2 Comparison with ad hoc MPCs

Table 57 shows the *ad hoc*-MPCs that existed for the twelve compounds investigated in this report. We have compared *ad hoc* values for water and soil with the ERLs derived in this report. In total, six new derived ERLs were lower than their existing *ad hoc* values. *Ad hoc*-MPCs based on ecotoxicological data are usually derived with stricter assessment factors to compensate for the less

intensive search for data. The general expectation would be that a more thorough MPC derivation (this report) would not lead to lower MPCs. However, since MPC derivation integrates human exposure as well, the explanation is often more complex. Explanation for the lower MPC_{water} values are given in the following. It should be noted that a comparison is sometimes hampered by the fact that the derivation of *ad hoc*-MPCs is not always well documented.
MPC_{water} for pentaBDE has lowered most probably since a much lower human toxicological risk limit was used for the current ERL derivation. The human risk limit used for the current *ad hoc*-MPC is unknown. The MPC_{water} for benzo[*b*]fluoranthene is only slightly lower than both *ad hoc*-MPC values; the difference is within a factor of two.

The MPC_{water} for DNOC (a plant protection product) has now been taken equal to the legally binding DW standard of 0.1 $\mu g.L^{-1}$ while this was not done for the *ad hoc*-MPC (based on ecotoxicological data).
The MPC_{water} for epichlorohydrin and 1,2-dibromoethane are now based on drinking-water consumption. For epichlorohydrin, the lowest *ad hoc*-MPC was probably based on ecotoxicological data, while the MPC in this report is based on a legally binding standard for drinking-water (CD 98/83/EC; EC, 1998). The *ad hoc*-MPC for 1,2-dibromoethane was based on ecotoxicological data, while the current MPC is based on a maximum contribution of 10% to the TDI by drinking of water. Due to the carcinogenic properties of 1,2-dibromoethane, this gives an MPC_{water} which is roughly a factor of 2700 lower.
The MPC_{water} for ethinylestradiol is much lower than both *ad hoc*-MPCs. This is caused by the fact that for *ad hoc*-MPC derivation a quick screening of literature is performed, while the MPC derived in this report is based on all retrieved ecotoxicity data (including the most recent). In recent years many aquatic toxicity studies with ethinylestradiol have been performed, which have revealed effects on reproduction of fish at very low levels. These studies were not addressed in the *ad hoc* procedure.
The MPC_{water} for 3,3'-dichlorobenzidine derived in this report is a factor of 50 lower than the *ad hoc*-MPC value. A slightly higher human risk limit (TL_{hh}) used for the derivation of the *ad hoc*-MPC (a factor of 2), means that a difference of a factor of 100 should be explained via other mechanisms. This is caused by the fact that human fish consumption according to WFD guidance is 115 $g.d^{-1}$, while a consumption rate of 11 $g.d^{-1}$ is used in the derivation of the *ad hoc*-MPC. Further, in the current MPC_{water}, only 10% of the TL_{hh} is allowed to be caused by a water concentration (via fish consumption). In the calculation of the *ad hoc*-MPC for 3,3'-dichlorobenzidine, the TDI was 'filled' for 92% via exposure to surface water. Hence, differences in TL_{hh}, fish consumption rate and the contribution of exposure routes that fill up TL_{hh}, explain the difference between both MPCs.

The only MPC_{soil} that is lower than the *ad hoc*-MPC, is the MPC_{soil} for ethinylestradiol. Toxicity data for soil organisms were lacking and the MPC_{soil} was derived using the MPC_{water} and equilibrium partitioning. The dominant route of ethinylestradiol into the environment is: human intake → excretion → sewage system (toilet) → sewage treatment plant → surface water. The MPC_{soil} is relatively low, since the MPC_{water} that is used to calculate the MPC_{soil}, is based on reproductive effects on vertebrates (fish), which occur at very low concentrations. Since it can not be excluded that higher organisms (e.g. amphibians) in terrestrial ecosystems become directly exposed to ethinylestradiol (should it end up in soil) we propose to maintain the MPC_{soil}.

9.3 ERLs derived in this report

Table 60 to Table 63 present all environmental risk limits that have been derived in this report. Please mind that the units (given in the header of each column) in Table 60 (NC) differ between the compartments. NC_{water}, NC_{marine}, $NC_{groundwater}$ and NC_{soil} are presented in $ng.L^{-1}$ or $ng.kg^{-1}$; while $NC_{sediment}$ and $NC_{marine\ sediment}$ are given in $\mu g.kg^{-1}$. All MPC values (Table 61) and MAC_{eco} values (Table 63) are given in $\mu g.L^{-1}$ or $\mu g.kg^{-1}$. All SRC_{eco} values (Table 62) are shown in $mg.L^{-1}$ or $mg.kg^{-1}$.

Table 60. Negligible concentrations (NC_{comp}) for twelve substances.

Compound	NC_{water} [ng.L^{-1}]	$NC_{sediment}$ [µg kg_{dw}^{-1}]	NC_{marine} [ng.L^{-1}]	$NC_{marine,\ sediment}$ [µg kg_{dw}^{-1}]	NC_{soil} [ng.kg_{dw}^{-1}]	$NC_{groundwater}$ [ng.L^{-1}]
pentaBDE	2.9×10^{-7}	18	2.9×10^{-7}	3.7	0.0043	0.0091
p-*tert*-octylphenol	1.2	0.20	0.12	0.020	190	1.2
benzo[*b*]fluoranthene	0.17[a]	8.1	0.017[a]	0.81	4.0[e]	0.17
isodrin	–[b]	–[c]		–[c]	–	–
DNOC	1	–[c]	–[d]	–[c]	1700	10
aniline	15	–[c]	1.5	–[c]	1800	15
epichlorohydrin	1.0[e]	–[c]	0.65	–[c]	9.4	1.0[e]
1,2-dibromoethane	0.018[e]	–[c]	0.033[e]	–[c]	0.12[e]	0.018[e]
ethinylestradiol	1.6×10^{-4}	–[c]	1.6×10^{-5}	–[c]	0.021	1.6×10^{-4}
methyl bromide	32	–[c]	3.2	–[c]	25	32
6PPD	4.8	8.5	0.48	0.85	8600	4.8
3,3'-dichlorobenzidine	5.2×10^{-5} [e]	0.33	5.2×10^{-8} [e]	0.033	0.029[e]	0.0015[e]

NCs in soil and sediment are expressed in $mg.kg^{-1}$ dry weight Dutch standard soil or sediment, respectively.
[a]Preliminary NC value, since EU_RAR is not yet finalised.
[b]NC not derived since the MPC was not derived, but the MPC is a standard set in 88/347/EEC (EC, 1988; daughter directive of 76/464/EC; EC, 1976) four the sum of four drins.
[c]Derivation of $MPC_{sediment}$ was not triggered for this substance (log $K_{p,\ susp\text{-}water}$ <3).
[d]No NC derived since MPC_{marine} was not derived. MPC_{marine} was not derived due to lack of data.
[e]This standard is derived from a human toxicological risk limit based on a cancer risk of $1{:}10^{-6}$ after life-long exposure.

Table 61. Maximum permissible concentrations (MPC_{comp}) for twelve substances.

Compound	MPC_{water} [µg.L^{-1}]	$MPC_{sediment}$ [µg kg_{dw}^{-1}]	MPC_{marine} [µg.L^{-1}]	$MPC_{marine,\ sediment}$ [µg kg_{dw}^{-1}]	MPC_{soil} [µg.kg_{dw}^{-1}]	$MPC_{groundwater}$ [µg.L^{-1}]	MPC_{air} [µg.m^{-3}]
pentaBDE	2.9×10^{-8}*	1800	2.9×10^{-8}*	370	4.3×10^{-4}	9.1×10^{-4}	–[d]
p-*tert*-octylphenol	0.12*	20	0.012*	2.0	19	0.12	–[d]
benzo[*b*]fluoranthene	0.017[a]*	810	0.0017[a]*	81	0.40[h]	0.017	–[d]
isodrin	0.010[b]	–[c]	0.0050[b]	–[c]	–	–	–[d]
DNOC	0.1	–[c]	–[g]	–[c]	170	1	–[d]
aniline	1.5	–[c]	0.15	–[c]	180	1.5	1[e]
epichlorohydrin	0.10[h]	–[c]	0.065	–[c]	0.94	0.10[h]	0.8[e,f,h]
1,2-dibromoethane	0.0018[h]	–[c]	0.0033[h]	–[c]	0.012[h]	0.0018[h]	0.0020[e,h]
ethinylestradiol	1.6×10^{-5}	–[c]	1.6×10^{-6}	–[c]	0.0021	1.6×10^{-5}	–[d]
methyl bromide	3.2	–[c]	0.32	–[c]	2.5	3.2	100[e]
6PPD	0.48	850	0.048	85	860	0.48	–[d]
3,3'-dichlorobenzidine	5.2×10^{-6} [h]	33	5.2×10^{-9} [h]	3.3	0.0029[h]	1.5×10^{-4} [h]	2.0×10^{-4} [e,f,h]

MPCs in soil and sediment are expressed in $mg.kg^{-1}$ dry weight Dutch standard soil or sediment, respectively.
[a]Preliminary MPC value, since EU_RAR is not yet finalised.
[b]Standard set in 88/347/EEC (EC, 1988; daughter directive of 76/464/EC; EC, 1976) four the sum of four drins.
[c]Derivation of $MPC_{sediment}$ was not triggered for this substance (log $K_{p,\ susp\text{-}water}$ <3).
[d]Non-volatile compound, ecotoxicological data for exposure via air were not retrieved and a human toxicological risk limit for chronic inhalation exposure has not been derived.
[e]Preliminary MPC value, limited experience with methodology of ERL derivation.
[f]Ecotoxicological data for exposure via air were not found.
[g]Not determined due to lack of data.
[h]This standard is derived from a human toxicological risk limit based on a cancer risk of $1{:}10^{-6}$ after life-long exposure.
*An AA-EQS proposal is also available in the draft (daughter) Directive COM (2006) 397 (see section 9.4).

Table 62. Serious risk concentrations for the ecosystem (SRC_{eco}) for twelve substances.

Compound	$SRC_{eco, water}$ [$mg.L^{-1}$]	$SRC_{eco, sediment}$ [$mg\ kg_{dw}^{-1}$]	$SRC_{eco, marine}$ [$mg.L^{-1}$]	$SRC_{eco, marine, sediment}$ [$mg\ kg_{dw}^{-1}$]	$SRC_{eco, soil}$ [$mg.kg_{dw}^{-1}$]	$SRC_{eco, groundwater}$ [$mg.L^{-1}$]
pentaBDE	0.0060	40	0.0060	40	154	0.0060
p-*tert*-octylphenol	0.041	6.5	0.041	6.5	6.5	0.041
benzo[*b*]fluoranthene	1.7×10^{-4}	8.3	1.7×10^{-4}	8.3	8.3	1.7×10^{-4}
isodrin	–	–[a]	–	–[a]	–	–
DNOC	1.8	–[a]	1.8	–[a]	19	1.8
aniline	5.5	–[a]	5.5	–[a]	27	5.5
epichlorohydrin	3.1	–[a]	3.1	–[a]	4.5	3.1
1,2-dibromoethane	0.79	–[a]	0.79	–[a]	3.2	0.79
ethinylestradiol	2.4×10^{-6}	–[a]	2.4×10^{-6}	–[a]	3.1×10^{-4}	2.4×10^{-6}
methyl bromide	0.18	–[a]	0.18	–[a]	0.13	0.18
6PPD	0.021	37	0.021	37	37	0.021
3,3'-dichlorobenzidine	0.096	55	0.096	55	55	0.096

[a]Derivation of $MPC_{sediment}$ was not triggered for this substance (log $K_{p, susp-water}$ <3), therefore SRC_{eco} was not derived.

Table 63. Maximum acceptable concentrations (MAC_{eco}) for twelve substances.

Compound	MAC_{eco} [$\mu g.L^{-1}$]
pentaBDE	n.p.*
p-*tert*-octylphenol	0.12**
benzo[*b*]fluoranthene	n.p.*
isodrin	n.d.
DNOC	0.66
aniline	1.5
epichlorohydrin	6.5
1,2-dibromoethane	0.40
ethinylestradiol	0.56
methyl bromide	7.0
6PPD	0.48
3,3'-dichlorobenzidine	0.058

n.d. = not derived.
n.p. = not possible to derive a standard.
*Equal to MAC-EQS in draft (daughter) Directive COM (2006) 397 (see section 9.4).
**Draft (daughter) Directive COM (2006) 397

9.4 Comparison of MPCs with EQS proposals from draft (daughter) Directive

Table 64 shows the EQS values proposed in the most recent version of the draft (daughter) Directive 'on environmental quality standards and pollution control in the field of water policy and amending Directive 2000/60/EC' (EC, 2006a).

- The MPC_{water} and MPC_{marine} for pentaBDE derived in this report are lower than the risk limits (AA-EQS) proposed in the draft EU Directive. The difference is explained by the use of a lower human risk limit in this report compared with the value used by the drafters of the WFD fact sheets. See section 4.1.3 for a more detailed explanation.
- The MPC_{water} and MPC_{marine} for p-*tert*-octylphenol proposed in this report are equal to the EQSs proposed in the draft EU Directive.
- The draft EU Directive proposes a sum standard for benzo[*b*]fluoranthene and benzo[*k*]fluoranthene of 0.03 $\mu g.L^{-1}$. The MPC_{water} proposed for benzo[*b*]fluoranthene (not a sum standard) is 0.017 $\mu g.L^{-1}$, a value which is derived from the draft EU-RAR. Since in the draft EU-RAR, the PNEC for benzo[*k*]fluoranthene is also 0.17 $\mu g.L^{-1}$ and the toxic unit (TU) approach is followed, the sum standard for both compounds would also be 0.17 $\mu g.L^{-1}$. Note that the draft EU-RAR does not actually propose a sum standard, this was put forward only for

reasons of comparison. It can be concluded that the derived MPC_{water} for benzo[*b*]fluoranthene is less than a factor of two lower than the EQS proposal.

Note that the AA-EQS values in the draft Directive for 'inland waters' and 'other surface waters' are equal, while the MPC_{marine} for benzo[*b*]fluoranthene derived in this report is a factor of 10 lower than the MPC_{water} (MPC for freshwater). The reason for this difference is that the WFD fact sheet underlying the AA-EQS values concludes that sufficient ecotoxicological data was available to conclude that marine organisms are not more sensitive to benzo[*b*]fluoranthene. However, the MPC values are copied from the draft EU-RAR, in which it was concluded that not enough toxicity data for specific marine taxa were available to apply a reduced assessment factor.

Table 64. EQS proposals for three WFD prioritised substances, cited from draft daughter Directive COM (2006) 397 (EC, 2006a).

Compound	AA-EQS inland surface water [µg.L^{-1}]	AA-EQS other surface waters [µg.L^{-1}]	MAC-EQS [µg.L^{-1}]
pentaBDE	0.0005	0.0002	n.a.
p-*tert*-octylphenol	0.1	0.01	n.a.
benzo[*b*]fluoranthene	0.03[a]	0.03[a]	n.a.

n.a. = not applicable, according to draft (daughter) Directive COM (2006) 397.
[a]EQS applies to Σ of benzo[*b*]fluoranthene and benzo[*k*]fluoranthene.

Acknowledgements

Mrs. A.J. van Middelaar is gratefully acknowledged for her assistance. The content of this report has been discussed by the members of the scientific advisory group (WK-INS), who are acknowledged for their contribution and comments. The scientific advisory group provides a non-binding scientific comment on the final draft of a report in order to advise the steering committee of the project 'International and National environmental quality standards for Substances in the Netherlands' (INS) on the scientific merits of the report.

References

Anonymus. 2003. Regeling inzake milieukwaliteitseisen voor het Scheldebekken. Den Haag: Sdu Uitgevers. Staatscourant nr. 28. p. 23.

Anonymus. 2004. Substance Data Sheet: (5) Pentabromodiphenylether (penta-BDE). Schmallenberg, Germany: Fraunhofer Institute Molecular Biology and Applied Biology. Report no. Draft of 010304. 12 pp.

Anonymus. 2005a. Environmental Quality Standards (EQS) Substance Data Sheet. Priority substance No. 25. Octylphenols (para-tert-octylphenol). Brussels, Belgium: Report no. Final. 18 pp.

Anonymus. Hazardous Substances Data Bank [Web Page] (Available at http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~Z57mxx:1) Accessed: 2005b.

Anonymus. Syracuse Research Corporation. Physprop database [Web Page] (Available at http://www.syrres.com/esc/physdemo.htm) Accessed: June 10, 2005c.

Anonymus. RIZA (Institute for Inland Water Management and Waste Water Treatment). Normen voor het waterbeheer. Tabellen [Web Page] (Available at http://www.rijkswaterstaat.nl/rws/riza/wateremissies/Thema/Normen_voor_het_waterbeheer/tabellen.html) Accessed: 2006a.

Anonymus. RIZA (Institute for Inland Water Management and Waste Water Treatment). *Normen zoeksysteem* [Web Page] (Available at http://www.rijkswaterstaat.nl/rws/riza/wateremissies/Thema/Normen_voor_het_waterbeheer/normen.php) Accessed: 2006b.

Anonymus. SPARC on-line calculator v3.1 [Web Page] (Available at http://ibmlc2.chem.uga.edu/sparc/index.cfm) Accessed: 2006c.

Anonymus. US EPA. High Production Volume (HPV) Challenge Program. Robust summaries and test plans [Web Page] (Available at http://cfpub.epa.gov/hpv-s/) Accessed: Oct. 20, 2006d.

Aldenberg T, Jaworska JS. 2000. Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicol Environ Saf 46: 1-18.

Andersen HR, Hansen M, Kjoholt J, Stuer-Lauridsen F, Ternes T, Halling-Sorensen B. 2005. Assessment of the importance of sorption for steriod estrogens removal during activated sludge treatment. Chemosphere 61: 139-146.

Andersen HR, Kjoholt J, Hansen M, Stuer-Lauridsen F, Dueholm Blicher T, Ingerslev F, Halling-Sorensen B. 2004 . Degradation of estrogens in sewage treatment processes. Denmark: Danish Environmental Protection Agency. Report no. 899. 61 pp.

Andersen HR, Wollenberger L, Halling-Sřrensen B, Kusk KO. 2001. Development of copepod nauplii to copepodites - a parameter for chronic toxicity including endocrine disruption. Environ Toxicol Chem 20: 2821-2829.

Anonymus. 1998. Besluit van 23 april 1998, houdende Warenwetbesluit Azo-kleurstoffen. 's-Gravenhage, the Netherlands: Sdu Uitgevers. Report no. 1998 339. 25 pp.

Anonymus. 2003. Besluit van 27 juni 2003 tot wijziging van het Warenwetbesluit Azo-kleurstoffen in verband met het beperken van de handel in en het gebruik van bepaalde gevaarlijke stoffen en preparaten. 's-Gravenhage, the Netherlands: Sdu Uitgevers. Report no. 2003 296. 5 pp.

Appleton HT, Sikka HC. 1980. Accumulation, elimination and metabolism of dichlorobenzidine in the bluegill sunfish. Environ Sci Technol 14: 50-54.

ARCEM. 2003. Hormonwirksame Stoffe in Österreichs Gewässer - Ein Risiko? Wien, Austria: Umweltbundesamt GmbH. Report no. ISBN 3-85457-695-1. 462 pp.

Arildskov NP, Pedersen PG, Albrechtsen H-J. 2001. Fate of the herbicides 2,4,5-T, atrazine and

DNOC in a shallow, anaerobic aquifer investigated by in sity passive diffusive emitters and laboratory batch experiments. Ground Water 39: 819-830.
ATSDR. 1992. Bromomethane. Agency for Toxic Substances and Disease Registry. Report no. TP-91/06. 104 pp.
ATSDR. 1998. 3,3'-Dichlorobenzidine (Update). Atlanta, Georgia, USA: Agency for Toxic Substances and Disease Registry. 145 pp.
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. Report no. 711701025. 297 pp.
Banerjee S, Sikka HC, Gray R, Kelly CM. 1978. Photodegradation of 3,3'-Dichlorobenzidine. Environ Sci Technol 12: 1425-1427.
Banerjee S, Yalkowsky SH, Valvani SC. 1980. Water solubillity and octanol/water partition coefficient of organics. Limitations of the solubility-partition coefficient correlation. Environ Sci Technol 14: 1227-1229.
Beek MA. 1999. Overzicht van ad hoc MTR's voor water. Lelystad: Institute for Inland Water Management and Waste Water Treatment. Report no. 99.046X. 23 pp.
Beek MA. 2002. Ad hoc MTR's voor de stoffen uit de Richtlijn 76/464/EEG. Lelystad: Institute for Inland Water Management and Waste Water Treatment. Report no. 2002.106X. 62 pp.
Belfroid AC, Van der Horst A, Vethaak AD, Schäfer AJ, Rijs GBJ, Wegener J, Cofino WP. 1999. Analysis and occurence of estrogenic hormones and their glucuronides in surface water and waste water in The Netherlands. Sci Total Environ 225: 101-108.
BioByte. 2006. BioLoom [computer program]. version 1.5. Claremont, CA, USA: BioByte Corporation.
Bontje D, Traas TP, Mennes W. 2005. A human exposure model to calculate harmonized risk limits. Bilthoven, the Netherlands: National Institute for Public Health and Environmental Protection. Report no. 601501022. 115 pp.
Boyd SA, Kao C-W, Suflita JM. 1984. Fate of 3,3'-dichlorobenzidine in soil: persistence and binding. Environ Toxicol Chem 3: 201-208.
Braekevelt E, Tittlemier SA, Tomy GT. 2003. Direct measurement of octanol-water partition coefficients of some environmentally relevant brominated diphenyl ether congeners. Chemosphere 51: 563-567.
Briggs GG. 1981. Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the Parachor. J Agric Food Chem 29: 1050-1059.
Broholm MM, Tuxen N, Rügge K, Bjerg PL. 2001. Sorption and degradation of the herbicide 2-Methyl-4,6-dinitrophenol under aerobic conditions in a sandy aquifer in Vejen, Denmark. Environ Sci Technol 35: 4789-4797.
Brooke D, Johnson I, Mitchell R, Watts C. 2005. Environmental risk evaluation report: 4-tert-octylphenol. Bristol, UK: Environment Agency. Report no. ISBN 1 84432 410 9. 205 pp.
Brooke LT. 1991. Results of freshwater exposures with the chemicals atrazine, biphenyl, butachlor, cabaryl, carbazole, dibenzofuran, 3,3'-dichlorobenzidine, dichlorovos, 1,2-epoxyethylbenzene (styrene oxide), isophorone, isopropalin, oxychlordane, pentachloroanisole, propoxur (baygon), tetrabromobisphenol A, 1,2,4,5-tetrachlorobenzene, and 1,2,3-trichloropropane to selected freshwater organisms. Superior, WI, USA: University of Wisconsin-Superior, Lake Superior Research Institute. 109 pp.
Canton JH, Wegman RCC, Mathijssen-Spiekman EAM, Wammes JY. 1980. Hydrobiologisch-toxicologisch onderzoek met methylbromide. Bilthoven: RIVM. Report no. 105/80 CBS VI/RA.
Clara M, Strenn B, Sracevic E, Kreuzinger N. 2004. Adsorption of bisphenol-A, 17beta-estradiol and 17alhpha-ethinylestradiole to sewage sludge. Chemosphere 56: 843-851.

Crommentuijn T, Kalf DF, Polder MD, Posthumus R, Van de Plassche EJ. 1997. Maximum permissible concentrations and negligible concentrations for pesticides. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601501 002. 174 pp.

CSTEE. 1999. Opinion on Human and Wildlife health Effects on Endocrine Disrupting Chemicals, with emphasis on Wildlife and in Ecotoxicology Test Methods. Brussels. Belgium: EC, DG XXIV, Scientific Committee on Toxicity, Ecotoxicity and the Environment. 95 pp.

CTB. Board for the authorisation of pesticides. *Pesticides database* [Web Page] (Available at http://www.ctb.agro.nl/) Accessed: 2005a.

CTB. 2005b. Toelatingsbesluit betreffende Methylbromide 100 voor ruimteontsmetting. Wageningen, the Netherlands: Het College voor de toelating van bestrijdingsmiddelen. Report no. 6476 N.

De Bruijn J, Busser F, Seinen W, Hermens J. 1989. Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the 'slow-stirring' method. Environ Toxicol Chem 8: 499-512.

De Jong FMW, Posthuma-Doodeman CJAM, Verbruggen EMJ. 2007. Ecotoxicologically based environmental risk limits for several volatile aliphatic hydrocarbons. Bilthoven, The Netherlands: National Institute for Public Health and the Environment. Report no. 601782002. 217 pp.

De Winter-Sorkina R, Bakker MI, Wolterink G, Zeilmaker MJ. 2006. Brominated flame retardants: occurence, dietary intake and risk assessment. Bilthoven, The Netherlands: National Institute for Public Health and the Environment. Report no. 320100002. 85 pp.

Deneer JW, Sinnige TL, Seinen W, Hermens JLM. 1988. A quantitative structure-activity relationship for the acute toxicity of some epoxy compounds to the guppy. Aquat Toxicol 13: 195-204.

Dobbs RA, Wang LW, Govind R. 1989. Sorption of toxic organic compounds on wastewater solids: correlation with fundamental properties. Environ Sci Technol 23: 1092-1097.

Donaldson FP, Nyman MC. 2005. Sorption of benzidine and 3,3'-dichlorobenzidine to lake sediments. 1. Conceptualization and development of a multiparameter model. Environ Toxicol Chem 24: 1022-1028.

Dutka BJ, Kwan KK. 1981. Comparison of three microbial toxicity screening tests with the microtox test. Bull Environ Contam Toxicol 27: 753-757.

EC. 1975. Council Directive of 16 June 1975 concerning the quality required of surface water intended for the abstraction of drinking water in the Member States (75/440/EEC). Brussels, Belgium: European Commission. L 194. p. 26-31.

EC. 1976. Council Directive of 4 May 1976 on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community (76/464/EEC). Brussels, Belgium: European Commission. L 129.

EC. 1988. Council Directive (88/347/EEC) of 16 June 1998 amending Annex II to Directive 86/280/EEC on limit values and qualtity objectives for discharges of certain dangerous substances included in List I of the Annex to Directive 76/464/EEC. Brussels, Belgium: European Commission. L 158. p. 35-41.

EC. 1998. Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. Brussels, Belgium: European Commission. L 330. p. 32-54.

EC. 1999. 1999/164/EC: Commission Decision of 17 February 1999 concerning the non-inclusion of DNOC of active substance in Annex I to Council Directive 91/414/EEC and the withdrawal of authorisations for plant protection products containing this active substance (notified under document number C(1999) 332). Brussels, Belgium: European Commission. L 054. p. 21-22.

EC. 2000. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. Brussels, Belgium:

European Commission. L 327. p. 1-72.
EC. 2001. European Union Risk Assessment Report Diphenyl ether, pentabromo derivative, Volume 50. Hansen, B. G., Munn, S. J., Pakalin, S., Heidorn, C. J. A., Allanou, R., Scheer, S., Pellegrini, G., Vegro, S., Luotamo, M., De Bruijn, J., Berthault, F., Loonen, H., Vormann, K., Naughton, A., Anfossi, V., and Praderio, L. eds. Luxembourg: Office for Official Publications of the European Communities. Report no. EUR 19730. 282 pp.
EC. 2002. European Union Risk Assessment Report 4-Nonylphenol (branched) and nonylphenol, Volume 10. Hansen, B. G., Munn, S. J., De Bruijn, J., Pakalin, S., Luotamo, M., Berthault, F., Vegro, S., Heidorn, C. J. A., Pellegrini, G., Vormann, K., Allanou, R., and Scheer, S. eds. Luxemburg: Office for Official Publications of the European Communities. Report no. EUR 20387 EN. 227 pp.
EC. 2004a. European Union Risk Assessment Report aniline, Volume 50. Munn, S. J., Allanou, R., Aschberger, K., Berthault, F., De Bruijn, J., Musset, S., O'Connor, S., Pakalin, S., Pellegrini, G., Scheer, S., and Vegro, S. eds. Luxembourg: Office for Official Publications of the European Communities. Report no. EUR 21092. 222 pp.
EC. 2004b. EUSES 2.0, the European Union System for the Evaluation of Substances [computer program]. version 2.0.3. Bilthoven, The Netherlands: Prepared by the National Institute for Public Health and the Environment (RIVM) for the European Chemicals Bureau.
EC. 2006a. Proposal for a Directive of the European Parliament and of the Coucil on environmental quality standards and pollution control in the field of water policy and amending Directive 2000/60/EC. Brussels, Belgium: European Commission. COM(2006) 397 final. p. 1-25.
EC. 2006b. European Union Risk Assessment Report Coal-tar pitch, high temperature. Luxemburg: Office for Official Publications of the European Communities. Report no. draft.
EC-JRC. 2003. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commision 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.
ECB. 2000a. IUCLID Dataset - 1-chloro-2,3-epoxypropane. Ispra, Italy: EC. 94 pp.
ECB. 2000b. IUCLID Dataset - 3,3'-dichlorobenzidine. Ispra, Italy: EC. 56 pp.
ECB. 2000c. IUCLID Dataset - N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD). Ispra, Italy: EC. 40 pp.
ECB. European Chemicals Bureau. *ESIS - European chemical Substances Information System* [Web Page] (Available at http://ecb.jrc.it/) Accessed: Sept. 8, 2005.
Finizio A, Vighi M, Sandroni D. 1997. Determination of n-octanol/water partition coefficient of pesticide. Critical review and comparison of methods. Chemosphere 34: 131-161.
Freitag D, Ballhorn L, Geyer H, Korte F. 1985. Environmental hazard profile of organic chemicals. Chemosphere 14: 1589-1616.
Garten CT, Trabalka JR. 1983. Evaluation of models for predicting terrestrial food chain behaviour of xenobiotics. Environ Sci Technol 17: 590-595.
GDCh, German Chemical Society-BUA. 1989. 3,3'-Dichlorobenzidine. Weinheim, Germany: VCH Verlagsgesellscharft mbH. Report no. BUA 30. 70, 72 pp.
GDCh, German Chemical Society-BUA. 1992. Epichlorohydin (1-chloro-2,3,epoxypropane). Stuttgart Germany: S. Hirzel Wissenschaftliche Verlagsgesellschaft. Report no. BUA 90. 132 pp.
GDCh, German Chemical Society-BUA. 1998. N-Isopropyl-N'-phenyl-1,4-phenylene diamine (IPPD) and N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylene diamine (6PPD). Stuttgart, Germany: S. Hirzel. Report no. BUA 207 and BUA 208. 70, 72 pp.
GDCh, German Chemical Society-BUA. 1999. Tris(2-chloroethyl)phosphate (No. 20), 3,3'-

Dichorobenzidine (No. 30), Hexachloroethane (No. 34), 2-Chloro-4-nitroaniline (No. 43), 1,2-Dibromoethane (No. 66), Methallyl chloride (No. 109), Ethyl acrylate (No. 128), Tetramethyllead/Tetraethyllead (No. 130), Acrolein (No. 157), Thiourea (No. 179). Weinheim, Germany: VCH Verlagsgesellscharft mbH. Report no. BUA 223 (Supplementary reports VII).

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.

Goodwin KD, Varner RK, Crill PM, Oremland RS. 2001. Comsumption of troposheric levels of methyl bromide by C_1 compound-utilizing bacteria and comparison to saturation kinetics. Appl Environ Microbiol 67: 5437-5443.

Government of Canada. 1993. Canadian Environmental Protection Act. Priority substances list assessment report. 3,3-Dichlorobenzidine. Ottawa, Ontario, Canada: Minister of Supply and Services Canada. Report no. En40-215/15E. 17 pp.

Government of Canada. 1994. Canadian Environmental Protection Act. Priority substances list assessment report. Aniline. Ottawa, Ontario, Canada: Minister of Supply and Services. Report no. En40-215/35E. 30 pp.

Haderlein SB, Schwarzenbach RP. 1993. Adsorption of substituted nitrobenzenes and nitrophenols to mineral surfaces. Environ Sci Technol 27: 316-326.

Haderlein SB, Weissmahr KW, Schwarzenbach RP. 1996. Specific adsorption of nitroaromatic explosives and pesticides to clay minerals. Environ Sci Technol 30: 612-622.

Hansler R, Posthumus R. in prep. Indicatieve milieukwaliteitsnormen voor prioritaire stoffen. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503025.

Hansler R, Traas TP, Mennes WC. 2006. Handreiking voor de afleiding van indicatieve milieukwaliteitsnormen. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503024. 64 pp.

Harder, A. 2002. Assessment of the risk potential of reactive chemicals with multiple modes of toxic action. Thesis. Swiss Federal Institute of Technology (ETH) Zurich, pp.

Hertel RF, Kielhorn T. 1995. Methyl bromide. Environmental Health Criteria 166. Hanover: World Health Organisation (WHO). 324 pp.

Hildebrand C, Londry KL, Farenhorst A. 2006. Sorption and desorption of three endocrine disrupters in soils. J Environ Sci Health Part B Pestic Food Contam Agric Wastes 41: 907-921.

Hogan NS, Lean DRS, Trudeau VL. 2006. Exposures to estradiol, ethinylestradiol and octylphenol affect survival and growth of *Rana pipiens* and *Rana sylvatica* tadpoles. J Toxicol Environ Health Part A 69: 1555-1569.

Holthaus KIE, Johnson AC, Jürgens MD, Williams RJ, Smith JJL, Carter JE. 2002. The potential for estradiol and ethinylestradiol to sorb to suspended and bed sediments in some English rivers. Environ Toxicol Chem 21: 2526-2535.

Hurwitz AR, Liu ST. 1977. Determination of aqueous solubility and pKa values of estrogens. J Pharmaceut Sci 66: 624-627.

IARC. 1979. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Sex Hormones (II). Lyon, France : WHO. Report no. Volume 21. 583 pp.

IARC. 1983. IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. Polynuclear aromatic compounds, Part1, Chemical, Environmental and Experimental Data. World Health Organisation. Report no. Volume 32; ISBN 92 832 1532 X. 477 pp.

IARC. 1987a. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42. Lyon, France : WHO. Report no. Volume 1 to 42, Supplement 7. 440 pp.

IARC. International Agency for Research on Cancer. *Summaries & evaluations: Oestrogens, steroidal (group 1). Evidence for carcinogenicity to humans (sufficient). Supplement 7* [Web

Page] (Available at http://www.inchem.org/documents/iarc/suppl7/oestrogenssteroidal.html) Accessed: 1987b.
IARC. 1999a. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Re-evaluation of Some Organic Chemicals, Hydrazine, and Hydrogen Peroxide. Lyon, France : WHO. Report no. Volume 71. 1589 pp.
IARC. 1999b. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals. Lyon, France : WHO. Report no. Volume 15, Supplement 7.
INERIS. chimie.ineris.fr. *1,2-Dibromoethane* [Web Page] (Available at http://chimie.ineris.fr/en/lien/basededonnees/environnementale/recherche/dossiers.php?id=644) Accessed: 2005.
IPCS. 1984. Environmental Health Criteria - Epichlorohydrin. Geneva, Switzerland: World Health Organization. Report no. 33. 51 pp.
IPCS. 1996. Environmental Health Criteria - 1,2-Dibromoethane. Geneva, Switzerland: World Health Organization. Report no. 177. 148 pp.
Jafvert CT. 1990. Sorption of organic acid compounds to sediments: intial model development. Environ Toxicol Chem 9: 1259-1268.
JECFA. 2000. Estradiol-17-ß, progesterone and testosterone. Toxicological evaluation of certain veterinary drug residues in food. Geneva, Switserland: World Health Organization (WHO) - IPCS: INternation Programme on Chemical Safety. Report no. WHO food additives series 43 (http://www.inchem.org/documents/jecfa/jecmono/v43jec05.htm).
Jobling S, Casey D, Rodgers-Gray T, Oehlmann J, Schulte-Oehlmann U, Pawlowski S, Baunbeck T, Turner AP, Tyler CR. 2004. Comparative responses of molluscs and fish to environmental estrogens and an estrogenic effluent. Aquat Toxicol 66: 207-222.
Jürgens MD, Holthaus KIE, Johnson AC, Smith JJL, Hetheridge M, Williams RJ. 2002. The potential for estradiol and ethinylestradiol degradation in english rivers. Environ Toxicol Chem 21: 480-488.
Krijgsheld KR, Van der Gen A. 1986. Assessment of the impact of the emission of certain organochlorine compounds on the aquatic environment. Part III: Epichlorohydrin. Chemosphere 15: 881-893.
Kuriyama SN, Talsness CE, Grote K, Chahoud I. 2005. Developmental exposure to low-dose PBDE-99: effects on male fertility and neurobehaviour in rat offspring. Environ Health Perspec 113: 149-154.
Lahnsteiner F, Berger B, Grubinger F, Weismann T. 2005. The effect of 4-nonylphenol on semen quality, viability of gametes, fertilization succes, and embryo and larvae survival in rainbow *(Oncorhynchus mykiss*). Aquat Toxicol 297-306.
Lai KM, Johnson KL, Scrimshaw MD, Lester JN. 2000. Binding of waterborne steroid estrogens to solid phases in river and estuarine systems. Environ Sci Technol 34: 3890-3894.
Layton AC, Gregory BW, Seward JR, Schultz TW, Sayler GS. 2000. Mineralization of steroidal hormones by biosolids in wastewater treatment systems in Tennessee U.S.A. Environ Sci Technol 34: 3925-3931.
Lee LS, Nyman AK, Nyman MC, Jafvert C. 1997. Initial sorption of aromatic amines to surface soils. Environ Toxicol Chem 16: 1575-1582.
Lee LS, Strock TJ, Sarmah AK, Rao PSC. 2003. Sorption and dissipation of testosterone, estrogens and their primary transformation products in soils and sediment. Environ Sci Technol 37: 4098-4105.
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). Schmallenberg, Germany: Fraunhofer-Institute Molecular Biology and

Applied Biology. 47 pp.
Lide DR, Ed. 1997. Handbook of Chemistry and Physics. 78 ed. Boca Raton, USA: CRC Press LLC.
Liebig M, Egeler P, Oehlmann J, Knacker T. 2005. Bioaccumulation of ^{14}C-17α-ethinylestradiol by the aquatic oligochaete *Lumbriculus variegatus* in spiked artifical sediment. Chemosphere 59: 271-280.
Lobo RA, Stanczyk FZ. 1994. New knowledge in the physiology of hormonal contraceptives . Am J Obstet Gynecol 170: 1499-1507.
Luttik R, Linders J. 1990. DNOC (definitieve versie; M-75). Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 88/678801/064. 36 pp.
Länge R, Hutchinson TH, Croudace CP, Siegmund F, Schweinfurth H, Hampe P, Panter GH, Sumpter JP. 2001. Effects of the synthetic estrogen 17α-ethinylestradiol on the life-cycle of the fathead minnow (*Pimephales promelas*). Environ Toxicol Chem 20: 1216-1227.
Mackay D, Shiu W-Y, Ma K-C. Physical-chemical properties and environmental fate. Handbook. CD-ROM. 2000. Chapman & Hall/CRC*net*BASE.
MDL INformation Systems, Inc. 1997. ISIS™/Draw [computer program]. version 2.1.3.d.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1998a. Prevention of carcinogenic azo dyes in the Netherlands (Background report). Zoetermeer, The Netherlands: VROM. Report no. 1998/34B - Publicatiereeks Stoffen, Veiligheid, Straling. 90 pp.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1998b. Prevention of carcinogenic azo dyes in the Netherlands (Main report). Zoetermeer, The Netherlands: VROM. Report no. 1998/34A - Publicatiereeks Stoffen, Veiligheid, Straling. 50 pp.
Meylan W, Howard PH. 1992. Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ Sci Technol 26: 1560-1567.
Newman MC, Ownby DR, Mézin LCA, Powell DC, Christensen TRL, Lerberg SB, Anderson B-A. 2000. Applying species-sensitivity distributions in ecological risk assessment: assumptions of distribution type and sufficient numbers of species. Environ Toxicol Chem 19: 508-515.
Nyman MC, Haber KS, Kentämaa HI, Blatchley III ER. 2002. Photodechlorination of 3,3'-dichlorobenzidine in water. Environ Toxicol Chem 21: 500-506.
Nyman MC, Nyman AK, Lee LS, Nies LF, Blatchley III ER. 1997. 3,3'-Dichlorobenzidine transformation processes in natural sediments. Environ Sci Technol 31: 1068-1073.
O'Connor OA, Young LY. 1989. Toxicity and anaerobic biodegradability of substituted phenols under methanogenic conditions. Environ Toxicol Chem 8: 853-862.
OECD. 1995. SIDS Initial assessment report for SIAM 3. PHENOL, 4-(1,1,3,3-TETRAMETHYLBUTYL)-. Williamsburg, VI, USA: OECD. 54 pp.
OECD. 2002. SIDS Initial assessment report for 13th SIAM Methyl bromide. Paris, France: OECD. 31 pp.
OECD. 2004. SIDS Initial assessment report for SIAM 18. N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylendiamine (6PPD). Paris, France: OECD. 36 pp.
Okkerman PC, Van de Plassche EJ, Slooff W, Van Leeuwen CJ, Canton JH. 1991. Ecotoxicological effects assessment: a comparison of several extrapolation procedures. Ecotoxicol Environ Saf 21: 182-193.
OSPAR Commission. 2005. OSPAR background document on 4-(dimethylbutylamino)diphenylamine (6PPD). OSPAR Commission. Report no. 2005/228; ISBN 1-904426-63-8. 26 pp.
Park BJ, Kidd K. 2005. Effects of the synthetic estrogen ethinylestradiol on early life stages of mink frogs and green frogs in the wild and *in situ*. Environ Toxicol Chem 24: 2027-2036.
Parrott JL, Blunt BR. 2005. Life-cycle exposure of fathead minnows (*Pimephales promelas*) to an ethinylestradiol concentration below 1 ng/L reduces egg fertilization success and demasculinizes males. Environ Toxicol 20: 131-141.

Pascoe D, Carroll K, Karntanut M, Watts M. 2002. Toxicity of 17α-ethinylestradiol and bisphenol A to the freshwater cnidarian *Hydra vulgaris* . Arch Environ Contam Toxicol 43: 56-63.

Petterson I, Arukwe A, Lundstedt-Enkel K, Mortensen AS, Berg C. 2006. Persistent sex-reversal and oviducal agenesis in adult Xenopus (Silurana) tropicalis frogs following larval exposure to the environmental pollutant ethynylestradiol. Aquat Toxicol 79: 356-365.

Phernambucq AJW, Geenen JPW, Barreveld HL, Molegraaf P. 1996. Speuren naar sporen III. Lelystad, the Netherlands: RIZA, RIKZ. Report no. RIZA 96.035, RIKZ 96.016. 196 pp.

Radix P, Severin G., Schramm KW, Kettrup A. 2002. Reproduction disturbances of *Brachionus calcyflorus* (rotifer) for the screening of environmental endocrine disrupters. Chemosphere 47: 1097-1101.

RIVM. National Institute for Public Health and the Environment. *Risico's van stoffen* [Web Page] (Available at http://www.rivm.nl/rvs/XML_normen/NormSearchResult.jsp?stof=534-52-1&norm=milieukwaliteit) Accessed: Mar. 9, 2006.

Sabljić A, Güsten H, Verhaar H, Hermens J. 1995. QSAR modelling of soil sorption. Improvements and systematics of log K_{oc} vs. log K_{ow} correlations. Chemosphere 31: 4489-4514.

Sarmah AK, Northcott GL. 2006. Effect of organic carbon removal on sorption of steroid hormones by three New Zealand soils. In: Anonymus SETAC Europe.

Seki M, Yokota H, Matsubara H, Tsuruda Y, Maeda M, Tadokoro H, Kobayashi K. 2002. Effect of ethinylestradiol on the reproduction and induction of vitellogenin and testis-ova in medaka (*Oryzias latipes*). Environ Toxicol Chem 21: 1692-1698.

Sheng G, Johnston CT, Teppen BJ, Boyd SA. 2001. Potential contributions of smectite clays and organic matter to pesticide retention in soils. J Agric Food Chem 49: 2899-2907.

Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments. Athens, GA, USA: US-EPA. Report no. EPA-600/3-78-068. 49 pp.

Slooff W, Canton JH. 1983. Comparison of the susceptibility of 11 freshwater species to 8 chemical compounds. II. (Semi)chronic toxicity tests. Aquat Toxicol 4: 271-282.

Ten Hulscher ThEM, Van der Velde LE, Bruggeman WA. 1992. Temperature dependence of Henry's law constants for selected chlorobenzenes, polychlorinated biphenyls and polycylic aromatic hydrocarbons. Environ Toxicol Chem 11: 1595-1603.

Ternes T, Herrmann N, Bonerz M, Knacker T, Siegrist H, Joss A. 2004. A rapid method to measure the solid-water distribution coefiicient (K_d) for pharmaceuticals and musk fragrances in sewage sludge. Water Res 38: 4075-4084.

Thompson CM, McAllister WA, Forbis AD, Kaiser FE. 1979. Dynamic toxicity of Santoflex 13 (AB-78-121) to fathead minnows (*Pimephales promelas*). Flow-through bioassay final report. St. Louis, MI, USA: Monsanto (Performed at ABC Laboratories, Inc.). Report no. #21850-A/AB-780121B (Monsanto). Study of 12 pages, raw data included in Appendix 92 pages. 104 pp.

Tittlemier SA, Tomy GT. 2001. Vapor pressures of six brominated diphenyl ether congeners. Environ Toxicol Chem 20: 146-148.

Tomlin CDS. The e-Pesticide Manual (Twelfth Edition). CD-ROM. 2002. Version: 2.2. The British Crop Protection Council.

Umwelt Bundes Amt. 1987. Luftqualitätskriterien für ausgwählte Umweltkanzerogene. Berlin, Germany: Erich Schmidt Verlag. Report no. Berichte 2/87. 280 pp.

UNEP/WMO. 2002. Executive Summary, *Scientific Assessment of Ozone Depletion*. Scientific Assessment Panel of the Montreal Protocol on Substances that deplete the ozone layer. 20 pp.

US EPA. 2003. Summaries. 793-24-8. 1,4-Benzenediamine, N-(1,3-dimethylbutyl)-N'-phenyl-. US EPA, website High Production Volume Challange Program: US EPA. 34 pp.

US EPA. 2004. EPI Suite™ [computer program]. version 3.12. U.S. Environmental Protection Agency; Office of Pollution Prevention Toxics and Syracuse Research Company .

US EPA. US EPA. *Integrated Risk Information System* [Web Page] (Available at http://www.epa.gov/iris/subst/index.html) Accessed: 2007b.

Van der Heijden C, Janssen P, Heijna E. 1987. Samenvatting humaan-toxicologie: Methylbromide. Bilthoven, The Netherlands: National Institute for Public Health and the Environment.

Van Vlaardingen PLA, Traas TP, Wintersen AM, Aldenberg T. 2004. *E_TX* 2.0 A program to calculate hazardous concentrations and fraction affected, based on normally distributed toxicity data. Bilthoven: National Institute for Public Health and the Environment. Report no. 601501028. 68 pp.

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) – Revision 2007. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601782001. 146 pp.

Vethaak AD, Rijs GBJ, Schrap SM, Ruiter H, Gerritsen A, Lahr J. 2002. Estrogens and xeno-estrogens in the aquatic environment of the Netherlands. Occurence, potency and biological effects. Lelystad, The Netherlands: Dutch National Institute of Inland Water Management and Waste Water Treatment (RIZA) and the Dutch National Institute for Coastal and Marine Management (RIKZ). Report no. RIZA/RIKZ 2002.001.

Visser JT, Linders J. 1992. Methyl bromide (definitieve versie). Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 91/670104/011. 35 pp.

Weber EJ, Colón D, Baughman GL. 2001. Sediment-associated reactions of aromatic amines. 1. Elucidation of sorption mechanisms. Environ Sci Technol 35: 2470-2475.

Weissmahr KW, Haderlein SB, Schwarzenbach RP, Hany R, Nüesch R. 1997. *In situ* spectroscopic investigations of adsorption mechanisms of nitroaromatic compounds at clay minerals. Environ Sci Technol 31: 240-247.

WHO. 1998. Guidelines for Drinking-Water Quality - Second Edition - Volume 2 - Health Criteria and Other Supporting Information - Addendum. Geneva: World Health Organisation. Report no. WHO/EOS/98.1. 283 pp.

WHO. 2004. Epichlorohydrin in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. Geneva: World Health Organisation. 7 pp.

Yamamoto H, Liljestrand HM, Shimizu Y, Morita M. 2003. Effects of physical-chemical characteristics on the sorption of selected endocrine disrupters by dissolved organic matter surrogates. Environ Sci Technol `37: 2646-2657.

Ying G-G, Kookana RS. 2005. Sorption and degradation of estrogen-like-endocrine disrupting chemicals in soil. Environ Toxicol Chem 24: 2640-2645.

Ying G-G, Kookana RS, Dillon P. 2003. Sorption and degradation of selected five endocrine disrupting chemicals in aquifer material. Water Res 37: 3785-3791.

Young WF, Whitehouse P, Johnson I, Sorokin N. 2002. Proposed predicted no effect concentrations (PNECs) for natural and synthetic steroid oostrogens in surface waters. Report no. P2-T04/1.

Yu Z, Xiao B, Huang W, Peng P. 2004. Sorption of steriod estrogens to soils and sediments. Environ Toxicol Chem 23: 531-539.

Zeilmaker MJ, Kroese ED, Van Haperen P, Van Veen MP, Bremmer HJ, Van Kranen HJ, Wouters MFA, Janus JA. 1999. Cancer risk assessment of azo dyes and aromatic amines from garment and footwear. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503014. 51 pp.

Zeilmaker MJ, Van Kranen HJ, Van Veen MP, Janus JA. 2000. Cancer risk assessment of azo dyes and aromatic amines from tattoo bands, folders of paper, toys, bed clothes, watch straps and ink. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503019. 45 pp.

Zillioux EJ, Johnson IC, Kiparissis Y, Metcalfe CD, Wheat JV, Ward SG, Liu H. 2001. The sheepshead minnow as an *in vivo* model for endocrine disruption in marine teleosts: A partial

life-cycle test with 17α-ethynylestradiol. Environ Toxicol Chem 20: 1968-1978.
Zwolsman JJG, Bernhardi L, IJpelaar GF, van den Berg G.A. 2004. Bescherming drinkwaterfunctie - Bescherming van oppervlaktewater voor de drinkwatervoorziening onder de Europese Kaderrichtlijn Water. Rijswijk: VEWIN. Report no. 2004/43/4243. 48 pp.

Abbreviations

6PPD	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine
AA-QS	annual average quality standard
ADI	acceptable daily intake
AF	assessment factor
ag	analytical grade
a.i.	active ingredient
am	artificial medium
ATSDR	agency for toxic substances and disease registry
BCF	bioconcentration factor
BMF	biomagnification factor
BUA	advisory committee on existing chemicals of environmental relevance (German institution)
bw	body weight
CAS	chemical abstract service
CD	commission directive
CEPA	Canadian environmental protection act
CF	continuous flow system
c.i.	confidence interval
ClogP	log octanol/water partitioning coefficient, calculated by software program BioLoom
CMR	carcinogenic, mutagenic, reprotoxic
CSTEE	scientific committee on toxicity, ecotoxicity and the environment
CTB	college toelating bestrijdingsmiddelen – Dutch board for the authorisation of pesticides
d	days
DCB	3,3'-dichlorobenzidine
DG	directorate general
DNOC	2-methyl-4,6-dinitrophenol = 4,6-dinitro-ortho-cresol
dtw	dechlorinated tap water
dw	de-ionised water, dechlorinated water or distilled water dry weight
DW	drinking-water
DW standard	drinking-water standard
EC	European commission; effect concentration
ECB	European chemicals bureau
ECx	effect concentration at which an effect of x% is observed, generally EC10 and EC50 are calculated
EEC	European economic community (replaced by EU)
EHC	environmental health criteria
EINECS	European inventory of existing commercial chemical substances
ELS	early life stage
ESR	existing substances regulation
US EPA	environmental protection agency
EPI Suite	estimation programs interface (software program for calculation of physicochemical and fate parameters, distributed by Us EPA)
EqP	equilibrium partitioning

EQS	environmental quality standard
ERL	environmental risk limit
ESIS	European chemical substances information system
EU	European union
EU-RAR	European union-risk assessment report
EUSES	European union system for the evaluation of substances
F	flow through system
FHI	Fraunhofer Institute
GC	gas chromatography
h	hours
HC_x	hazardous concentration at which x percent of species is potentially affected
HPLC	high pressure liquid chromatography
HSDB	hazardous substances database
IARC	international agency for research on cancer
IF	intermittent flow system
INS	International and national environmental quality standards for substances in the Netherlands (In Dutch: (Inter)nationale Normen Stoffen)
IPCS	international programme on chemical safety
ISO	international organisation for standardisation
IUCLID	international uniform chemical information database
IUPAC	international union of pure and applied chemistry
JECFA	joint expert committee on food additives
LCx	effect concentration at which x% lethality is observed, generally LC50 and LC10 are calculated
LD50	dose that is lethal to 50% of the tested animals
lg	laboratory grade
LSC	liquid scintillation counting
LOEC	lowest observed effect concentration
MAC_{eco}	maximum acceptable concentration for ecosystems
MATC	maximum acceptable toxicant concentration
MlogP	log octanol/water partitioning coefficient, measured value selected by software program BioLoom
min	minutes
mo	months
MPC	maximum permissible concentration
MRL	minimum risk level
MS	mass spectrometry
NC	negligible concentration
NER	Nederlandse emissierichtlijn lucht
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
nw	natural water, such as lake water, river water, sea water, well water
oc	organic carbon
OECD	organisation for economic co-operation and development
om	organic matter
OSPAR	Olso-Paris convention
pa	pro analyse
PAH	polycyclic aromatic hydrocarbon
PCTHT	coal tar pitch – high temperature fraction

pentaBDE	pentabromo diphenyl ether
PNEC	predicted no effect concentration
ppt	parts per thousand[7] or parts per trillion
QS	quality standard
QSAR	quantitative structure activity relationship
R	renewal system
RAR	risk assessment report
RfD	reference dose
rg	reagent grade
rtw	reconstituted tap water: tap water with additional salts
rw	reconstituted water: (natural) water with additional salts
RIVM	national institute for public health and the environment
RIZA	institute for inland water management and waste water treatment
S	static
Sc	static, closed system
SEC	expertise centre for substances
SIDS	screening information data set
SMILES	simplified molecular input line entry system
sp.	species
SPARC	SPARC performs automatic reasoning in chemistry
SRC_{eco}	ecotoxicological serious risk concentration
STP	sewage treatment plant
susp	suspended particulate matter
SSD	species sensitivity distribution
TCA	tolerable concentration in air
TDI	tolerable daily intake
TERA	toxicology excellence for risk assessment
tg	technical grade
TGD	technical guidance document
TLC	thin layer chromatography
TL_{hh}	threshold limit for human health
TLm	median tolerance limit; also encountered as: median threshold limit
tw	tap water
UNEP	united nations environment programme
US	United States
UV	ultraviolet
VROM	ministry of housing, spatial planning and the environment
w	weeks
WFD	water framework directive
WHO	world health organisation
ww	wet weight
y	years

[7] Salinity is often expressed as ppt, in which case ‘ppt’ means parts per thousand (grams of chloride per kg of water).

Appendix 1 Aquatic toxicity data used for extrapolation

Contents

Table A1. 1. PentaBDE: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
algae	0.0046[a]	crustacea	0.014
crustacea	0.0053	pisces	>500
pisces	0.0089		

[a]Geometric mean of 0.0033 and 0.0065 mg.L^{-1} for *Selenastrum capricornutum*.

Table A1. 2. p-tert-Octylphenol; selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
algae	0.3	algae	1.1
crustacea	0.037[a]	algae	1.9
pisces	0.0061[b]	crustacea	0.16[c]
		crustacea	0.0133[d]
		pisces	0.54[e]
		pisces	0.23[f]
		pisces	0.65[g]
		pisces	0.27

[a]Lowest value (parameter growth) for *Daphnia magna*.
[b]Lowest value (parameter growth of fry) for *Oncorhynchus mykiss*.
[c]Geometric mean of 0.27 and 0.09 mg.L^{-1}, parameter mortality for *Daphnia magna*.
[d]Lowest value (parameter immobilisation) for *Gammarus pulex*.
[e]Geometric mean of 0.26, 0.6 and 1.0 mg.L^{-1}, parameter mortality for *Leuciscus idus*.
[f]Geometric mean of 0.45 and 0.12 mg.L^{-1}, parameter mortality for *Oncorhynchus mykiss*.
[g]LC50 is given as a range; presented is the geometric mean of upper and lower value of the range (0.45 and 0.94 mg.L^{-1}) parameter mortality for *Oryzias latipes*.
[h]Geometric mean of 0.29 and 0.25 mg.L^{-1}, parameter mortality for *Pimephales promelas*.

Table A1. 3. Benzo[b]fluoranthene: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
		crustacea	0.0042

Table A1. 4. Benzo[k]fluoranthene: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
pisces	0.00017[a]		

[a]Lowest value (parameter growth (length)) for *Brachydanio rerio*.

Table A1. 5. DNOC: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
bacteria	100	bacteria	6.2[g]
bacteria	10[a]	algae	74[h]
bacteria	16	protozoa	5.9[i]
bacteria	0.039	crustacea	2.7[j]
cyanobacteria	0.69[b]	crustacea	0.15
algae	100	crustacea	1.1
algae	1.0	insecta	0.32
algae	10	pisces	4.7[k]
algae	22[c]	pisces	0.29[l]
algae	16	pisces	0.066
protozoa	5.4	pisces	1.9
protozoa	5.4	pisces	0.18[m]
protozoa	30		
protozoa	0.012		
macrophyta	0.32		
coelenterata	0.32		
rotifera	0.55		
mollusca	0.032[d]		
crustacea	0.21[e]		
insecta	10		
pisces	0.18		
pisces	1.0		
pisces	0.1[f]		
amphibia	0.32		

[a]Lowest value (parameter growth) for *Pseudomonas fluorescens*.
[b]Geometric mean of 3.2 and 0.15 mg.L^{-1} for growth of *Microcystis aeruginosa*.
[c]Geometric mean of 13 and 36 mg.L^{-1} for growth of *Scenedesmus quadricauda*.
[d]Lowest value (parameter reproduction) for *Lymnea stagnalis*.
[e]Lowest value (parameter growth) for *Daphnia magna*.
[f]Lowest value (parameter mortality) for *Oryzias latipes*.
[g]Geometric mean of 6.6, 6.6, 6.3 and 5.5 mg.L^{-1} for luminescence of *Vibrio fischeri*.
[h]Geometric mean of 110 and 50 mg.L^{-1} for growth of *Scenedesmus subspicatus*.
[i]Geometric mean of 3.7 and 9.3 mg.L^{-1} for growth of *Tetrahymena pyriformis*.
[j]Geometric mean of 6.6, 8, 3.1, 2.0, 3.3, 5.1, 2.7, 2.3, 5.7 and 0.1 mg.L^{-1} for mortality and immobilisation of *Daphnia magna*.
[k]Lowest value (parameter circulation) for *Danio rerio*.
[l]Geometric mean of 0.23 and 0.36 mg.L^{-1} for mortality of *Lepomis macrochirus*.
[m]Geometric mean of 2.2, 1.9, 1.7, 1.3, 1.95, 1.54 and 2.7 mg.L^{-1} for mortality of *Pimephales promelas*.

Table A1. 6. Aniline: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
Algae	0.16	Algae	19
Algae	2	Algae	68
Algae	22	Crustacea	0.68
Crustacea	0.011[a]	Crustacea	2.3
Pisces	0.39	Crustacea	0.21[b]
Bacteria	250	Crustacea	0.1
Bacteria	24	Pisces	42.9[c]
Bacteria	130	Pisces	49
Bacteria	91	Pisces	22.1[d]
		Pisces	68.6
		Bacteria	<1
		Bacteria	53

[a]Geometric mean of 0.016, 0.004, 0.024 and 0.0102 mg.L^{-1} for *Daphnia magna*.
[b]Geometric mean of 0.17, 0.3, 0.16, 0.25 mg.L^{-1} for *Daphnia magna*.

[c]Geometric mean of 32 and 57.5 $mg.L^{-1}$ for *Danio rerio*.
[d]Geometric mean of 28.3, 10.6 and 36.2 $mg.L^{-1}$ for *Oncorhynchus mykiss*.

Table A1. 7. Epichlorohydrin: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [$mg.L^{-1}$]	taxonomic group	L(E)C50 [$mg.L^{-1}$]
bacteria	55	bacteria	670[a]
cyanobacteria	6.0	bacteria	316
protozoa	29	algae	24.2
protozoa	35	crustacea	11.9
protozoa	57	pisces	23
algae	10.7	pisces	27
algae	5.4	pisces	0.65
		pisces	36[b]

[a]Lowest value (test duration 15 minutes) for luminescence of *Vibrio fischeri*.
[b]Lowest value (test duration 48 h) for mortality of *Rasbora heteromorpha*.

Table A1. 8. 1,2-Dibromoethane: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [$mg.L^{-1}$]	taxonomic group	L(E)C50 [$mg.L^{-1}$]
pisces	5.81	algae	4
		bacteria	211.5
		coelenterata	50[a]
		crustacea	6.5
		crustacea	3.61
		pisces	0.04[b]
		pisces	4.8
		pisces	4.3
		pisces	32.1
		pisces	18[c]
		pisces	15[d]

[a]Lowest value (parameter mortality) for developing embryos/larvae of *Centropomus undecimalis*.
[b]Lowest value (parameter mortality) for developing embryos/larvae of *Centropomus undecimalis*.
[c]Lowest value (parameter mortality) for *Lepomis macrochirus*.
[d]Lowest value (parameter mortality) for *Micropterus salmoides*.

Table A1. 9. Ethinylestradiol: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [$mg.L^{-1}$]	taxonomic group	L(E)C50 [$mg.L^{-1}$]
algae	0.054	algae	12.4
rotifera	0.51	algae	0.84
mollusca	5.0×10^{-6}	cnidaria	3.8
crustacea	0.046	crustacea	0.088[e]
crustacea	10	crustacea	1.814
insecta	0.1	crustacea	0.84
pisces	2.0×10^{-5a}	crustacea	5.7
pisces	3.0×10^{-7b}	pisces	1.7
pisces	2.0×10^{-6c}	amphibia	0.56
pisces	1.6×10^{-7d}	amphibia	0.97[f]
pisces	4.4×10^{-5}		

[a]Lowest value (parameters reproduction and hatching) for *Cyprinodon variegatus*.
[b]Lowest value (parameters growth, egg production, no, of fertilised eggs and time to maturation) for *Danio rerio*.
[c]Lowest value (parameter reproduction) for *Oryzias latipes*.
[d]Lowest value (parameter fertility) for *Pimephales promelas*.

[e]Lowest value (parameter development for a 120 hour study) for *Acartia tonsa*.
[f]Geometric mean of 0.89, 0.82 and 1.24 mg.L^{-1}, parameter mortality, for *Rana pipiens*.

Table A1. 10. Methyl bromide: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
pisces	0.32	algae	5.0
pisces	0.1	algae	3.2
		crustacea	2.2
		pisces	0.8
		pisces	0.7

Table A1. 11. 6PPD: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
algae	0.22	algae	0.668
pisces	0.024	crustacea	0.23
		pisces	0.028
		pisces	0.45

Table A1. 12. 3,3'-Dichlorobenzidine: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
algae	0.32	bacteria	0.058
		algae	4.3
		crustacea	0.73
		crustacea	1.61
		pisces	3.3
		pisces	0.5
		pisces	1.57[a]

[b]Geometric mean of 2.08, 1.05 and 1.77 mg.L^{-1} for mortality of *Pimephales promelas*.

Appendix 2 Terrestrial toxicity data used for extrapolation

Contents

Table A2. 1. PentaBDE: selected terrestrial data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
nitrification	> 5.9	annelida	> 456
macrophyta	431		
macrophyta	55.2		

Table A2. 2. DNOC: selected terrestrial data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
processes	22.4[a]	annelida	65
enzymatic activity	16.9	annelida	20

[a]Geometric mean of 16.9 and 29.7 mg.kg$_{dw}^{-1}$ standard soil for inhibition of glucose respiration.

Table A2. 3. Aniline: selected terrestrial data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
		macrophyta	183[a]

[a]Lowest value of two results obtained for *Lactuca sativa*. Note that the choice for this result is taken over from the EU-RAR for aniline, in which the lowest EC50 from two tests with the same species was selected. In our opinion, taking the geometric mean of the two EC50 would have been the preferred data treatment in this case. However, in this case, the PNEC derivation from the EU-RAR should be copied and hence the lowest value of 33 mg.kg^{-1} in test soil (=183 mg/kg in Dutch standard soil) will be used for ERL derivation.

Table A2. 4. 1,2-Dibromoethane: selected terrestrial data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
fungi	3.29		

Table A2. 5. Methyl bromide: selected terrestrial data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
		macrophyta	8.6
		macrophyta	2.5
		macrophyta	8.2
		macrophyta	4.9
		macrophyta	12.1
		macrophyta	6.7
		macrophyta	7.1
		macrophyta	15.9

Appendix 3 Sediment toxicity data used for extrapolation

Contents

Table A3. 1. PentaBDE: selected sediment data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.kg^{-1}]	taxonomic group	L(E)C50 [mg.kg^{-1}]
annelida	18.2		
crustacea	37.0		
insecta	94.1[a]		

[a]Lowest value (parameter development rate) for *Chironomus riparius*.

Appendix 4 Air toxicity data used for extrapolation

Contents

Table A4. 1. 1,2-dibromoethane: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
fungi	424	insecta	10.2[a]
		insecta	0.243[b]
		insecta	0.9[c]
		insecta	3.0[d]
		insecta	3.0[e]
		insecta	2.6[f]
		insecta	2.8[g]
		insecta	13.5
		insecta	3.4[h]
		insecta	143.9
		insecta	2.2[i]

[a]Lowest value from a study with *Acanthoscelides obdectus* exposure times 6 hours.
[b]Most sensitive life-stage of *Callosobruchus chinensis*.
[c]Lowest value from a study with *Oryzaephilus surinamensis*.
[d]Lowest value from a study with *Rhyzopertha dominica* .
[e]Lowest value from two studies with *Sitophilus granarius*.
[f]Lowest value from a study with *Sitophilus oryza*.
[g]Lowest value from a study with *Stegobium paniceum*.
[h]Lowest value from two studies with *Tribolium confusum*.
[i]Lowest value from a study with *Zabrotes pectoralis*.

Table A4. 2. Methyl bromide: selected aquatic data for ERL derivation.

taxonomic group	NOEC or EC10 [mg.L^{-1}]	taxonomic group	L(E)C50 [mg.L^{-1}]
		insecta	4.2[a]
		insecta	0.851[b]
		insecta	1.67[c]
		insecta	2.18[d]
		insecta	31.7[e]
		insecta	7.1[f]
		insecta	4.4[g]
		insecta	5.5[h]
		insecta	3.4[i]
		insecta	4.8[j]
		insecta	4.2
		insecta	3.6[k]
		insecta	5.80[l]
		insecta	1.90[m]
		insecta	4.4[n]
		insecta	4[o]
		insecta	3.24[p]
		insecta	4.9[q]
		insecta	3.5[r]

[a]Lowest value from a study with *Acanthoscelides obdectus*.
[b]Lowest value from a study with *Callosobruchus chinensis* .
[c]Geomean of toxicity values from a study with *Corcyra cephalonica.*
[d]Geomean of toxicity values from two studies with *Cydia pomonella*.
[e]Geomean of toxicity values from two studies with *Ephestia kuehniella*.
[f]Lowest value of a study with *Maconellicoccus hirsutus*.
[g]Lowest values from a study with *Oryzaephilus surinamensis* .
[h]Lowest value from a study with *Plodia interpunctella*.
[i]Lowest value from a study with *Rhyzopertha dominica* .
[j]Lowest value from a study with *Sitophilus granarius*.
[k]Geomean of toxicity values from a study with *Sitophilus oryza*.
[l]Geomean from a study with *Sitophilus oryza.*
[m]Geomean of toxicity values from a study with *Sitotroga cerealella*.

[n]Lowest of toxicity values from a study with *Stegobium paniceum*.
[o]Lowest value from two studies with *Tenebroides mauritanicus*.
[p]Geomean of toxicity values from a study with *Tribolium castaneum*.
[q]Geomean of toxicity values from four studies with *Tribolium confusum* exposure 16 hours.
[r]Lowest value from a study with *Zabrotes pectoralis*.

Appendix 5 Information on aquatic toxicity

Contents

Legend

Species	organism used in the test.
Species properties	age, size, weight or life stage. ad = adult, emb = embryo, juv = juvenile.
A	Y = test substance analyzed in test solution. N = test substance not analyzed in test solution. field empty = no data.
Test type	CF = continuous flow, F= flow through, IF = intermittent flow, R = static with renewal, S = static.
Test compound	name of test chemical.
Purity	purity of the test compound: %active ingredient, ag = analytical grade, lg= laboratory grade, pa = pro analysis, rg = reagent grade, tg = technical grade.
Test water	am = artificial medium, asw = artificial seawater, de-ion w, dist w = distilled water, exp. stream = experimental stream, lw = lake water, nfs = natural filtered seawater, nw = natural water, nsw = natural sea water, rec w = reconstituted water, rec tw = reconsituted tap water (+additional salts), river w = river water, salt w = salt water, sw = sea water, syn w = synthetic water, tw = tap water.
pH	pH of test medium.
T	temperature during the test.
Hardness	hardness of test medium, expressed as mg $CaCO_3$ per litre.
Exposure time	h = hours, d = days, w = weeks, m = months, min. = minutes
Criterion	EC50 = lowest short term test result showing 50% mortality; LC50 = lowest short term test result showing 50% effect; NOEC = no observed effect concentration; LOEC = lowest observed effect concentration; ECx = effect concentration causing x% effect.
Test endpoint	the biological parameter investigated.
Value	test result; > and ≥ symbols = no effect observed at highest test concentration.
Notes	remarks to the summarised test result.
Reference	source of the study.

Table A5. 1. Acute toxicity of pentaBDE to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3.L^{-1}]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Crustacea															
Daphnia magna		Y		F						48 h	EC50	mortality	0.014	1	Cited in EC, 2001
Daphnia magna		Y		F						48 h	NOEC	mortality	0.0049		Cited in EC, 2001
Pisces															
Oncorhynchus mykiss				F						96 h	LC50	mortality	> Sw	2	Cited in EC, 2001
Oryzias latipes	ad; 0.13 g									48 h	LC50	mortality	>500	3	Cited in EC, 2001

Notes

1 It was noted in the test report that the effects could have been due to physical impairment rather than a direct toxic effect.
2 No deaths at highest test concentration of 21 µg.L^{-1}.
3 No deaths at highest test concentration of 500 mg.L^{-1}. Concentration of DMSO and a dispersing agent were above recommended values in EU test-method, i.e. 5 g.L^{-1} and 10 g.L^{-1} versus the recommended value of 100 mg.L^{-1}. The endpoint exceeds substance's solubility greatly.

Table A5. 2. Acute toxicity of p-tert-octylphenol to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$.L^{-1}]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Algae															
Scenedesmus subspicatus		N	S	4-tert-OP						72 h	EC50	growth rate	1.1		Cited in Brooke *et al*., 2005
Selenastrum capricornutum		N	S	4-tert-OP	'high'			24-25		96 h	EC50	growth rate	1.9		Cited in Brooke *et al*., 2005
Crustacea															
Daphnia magna		N		4-tert-OP						24 h	EC50		0.17		Cited in Brooke *et al*., 2005
Daphnia magna		Y	F	4-tert-OP	99.3		8.3-8.4	20		48 h	LC50	mortality	0.27		Cited in Brooke *et al*., 2005
Daphnia magna	neonates		S	4-OP			7.0-7.2	20-22		48 h	LC50	mortality	0.09		Cited in Brooke *et al*., 2005
Gammarus pulex	1st and 2nd instar	Y	R	4-tert-OP						96 h	EC50	immobilisation	0.0133		Cited in Brooke *et al*., 2005
Gammarus pulex	1st and 2nd instar	Y	R	4-tert-OP						96 h	EC50	mortality	0.0196		Cited in Brooke *et al*., 2005
Pisces															
Leuciscus idus	6 ± 2 cm	Y	R	4-tert-OP			7.5-7.9	20		96 h	LC50	mortality	0.26		Cited in Brooke *et al*., 2005
Leuciscus idus		N								48 h	LC50	mortality	0.6		Cited in Brooke *et al*., 2005
Leuciscus idus		N			95					96 h	LC50	mortality	1.0		Cited in Brooke *et al*., 2005
Oncorhynchus mykiss				4-tert-OP						24 h	LC50	mortality	0.45		Cited in Brooke *et al*., 2005
Oncorhynchus mykiss		Y	F	4-tert-OP	99.3			12		14 d	LC50	mortality	0.12		Cited in Brooke *et al*., 2005
Oryzias latipes	fert. to swim-up	N	S	4-tert-OP				25		17 d	LC50	mortality	0.45-0.94	1	Cited in Brooke *et al*., 2005
Pimephales promelas		Y	F	4-tert-OP	99.3		8.0-8.2	22		96 h	LC50	mortality	0.29		Cited in Brooke *et al*., 2005
Pimephales promelas										24 h	NOEC		0.15		Cited in Brooke *et al*., 2005
Pimephales promelas										96 h	LC50	mortality	0.25		Cited in Brooke *et al*., 2005

Notes

1 Test animals were embryos at day 0 and larvae at day 17.

Table A5. 3. Acute toxicity of benzo[b]fluoranthene to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [µg.L^{-1}]	Notes	Reference
Crustacea															
Daphnia magna	< 24 h	Y	S			am	7.8±0.2		250±30	48 h	EC50	immobility	>1.1	1	Bisson *et al*., 2000, cited in EC, 2006
Daphnia magna	4 d	N	S		97	nw	8		250	24 h	EC50	immobility	>1024	2	Wernersson and Dave, 1997, cited in EC, 2006
Daphnia magna	4 d	N	S		97	nw	8		250	24 h+2 h +2 h	EC50	immobility	4.2	3	Wernersson and Dave, 1997, cited in EC, 2006

Notes
1 Test performed in the dark.
2 Photoperiod was 16 h (artificial) light and 8 h darkness.
3 After 24 h PAH exposure 2 h UV irradiation (295-365 nm; peak 340 nm; intensity 370±20 µW/cm2) and a recovery period of 2 h; temperature 20°C; during UV-radiation and recovery 23°C.

Table A5. 4. Acute toxicity of benzo[k]fluoranthene to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [µg.L^{-1}]	Notes	Reference
Crustacea															
Daphnia magna	< 24 h	Y	S			am	7.8±0.2		250±30	48 h	EC50	immobility	>1.1	1	Bisson *et al*., 2000, cited in EC, 2006
Daphnia magna	<24 h	N	S			am	7.8		250	48 h	EC30	immobility	>1	1	Verrhiest *et al*., 2001, cited in EC, 2006
Daphnia magna	<24 h	N	S			am	7.8		250	48+2 h	EC50	immobility	>1	2	Verrhiest *et al*., 2001, cited in EC, 2006
Daphnia magna	<24 h	N	S			am	7.8		250	48 h	EC50	immobility	>1	3	Verrhiest *et al*., 2001, cited in EC, 2006
Daphnia magna	<24 h	N	S			am	7.8		250	48+2	EC90	immobility	>1	4	Verrhiest *et al*., 2001, cited in EC, 2006

Notes
1 Test performed in the dark.
2 48 h exposure in the dark followed by 2 h exposure to UV-A (365 nm, 247 µW.cm^{-2}).
3 Exposure under white light (2500 lux, 74-92 µW.cm^{-2}), 16 h light/8 h dark.
4 48 h exposure in white light (see 65) followed by 2 h exposure to UV-A (365 nm, 247 µW.cm^{-2}).

Table A5. 5. Acute toxicity of DNOC to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Scenedesmus subspicatus		N	S	DNOC		am	8.0	24	65	48 h	EC50	growth	110		Kühn and Pattard, 1990
Scenedesmus subspicatus	strain 86.81 SAG	N	S	DNOC		am				72 h	EC50	growth	50		Gälli *et al*., 1994
Protozoa															
Tetrahymena pyriformis		N	S	DNOC		am	7.3	27	7.3	60 h	EC50	growth	3.7		Schultz *et al*., 1986; Schultz *et al*., 1996; Schultz, 1997; Bearden and Schultz, 1998;Schultz *et al*., 1999
Tetrahymena pyriformis		N	S	DNOC	≥95	am	7.3	27	7.3	48 h	EC50	growth	9.3	1	Cajina-Quezada and Schultz, 1990
Crustacea															
Daphnia magna	<24 h, 0.315-0.630 mm	N	S	DNOC		tw	7.6-7.7	20-22	286	24 h	EC50	immobility	6.6		Bringmann and Kühn, 1977
Daphnia magna	<24 h	N	S	DNOC		nw	7.5	23	67	48 h	EC50	immobility	8.0		Bringmann and Kühn, 1959
Daphnia magna	<24 h		S	DNOC		rww	8.3	22	173	48 h	LC50	mortality	3.1		LeBlanc, 1980
Daphnia magna	<24 h, Strauss, IRCHA	N	S	DNOC		am	8.0±0.2	20	250.2	24 h	EC50	immobility	2.0	2	Bringmann and Kühn, 1982
Daphnia magna		Y	S	DNOC						48 h	LC50	mortality	3.3		Hermens *et al*., 1984
Daphnia magna	<72 h	N	S	DNOC	> 95	recw	7.8-8.2	20	200	24 h	EC50	immobility	5.1		Devillers *et al*., 1987
Daphnia magna	6-24 h	N	S	DNOC		am	8	20	240	48 h	EC50	immobility	2.7		Kühn *et al*., 1989
Dapnhia magna	<24 h, IRCHA	N	S	DNOC		am	8	25	250	24 h	EC50	immobility	2.3		Kühn *et al*., 1989
Dahpnia magna		N	S	DNOC	≥ 99					24 h	EC50		5.7		Luttik and Linders, 1990
Dahpnia magna		N	S	DNOC		am				24 h	EC50	immobility	0.1	3	Gälli *et al*., 1994
Daphnia pulex	1st instar	N	S	DNOC	100	rdw	7.1	21	44	48 h	EC50		0.145		Mayer and Ellersieck, 1986
Gammafus fasciatus	mature	N	S	DNOC	100	rdw	7.1	21	44	96 h	LC50	mortality	1.1		Mayer and Ellersieck, 1986
Insecta															
Pteronarcys californica	2nd y class	N	S	DNOC	100	rdw	7.1	15	44	96 h	LC50	mortality	0.32		Sanders and Cope, 1968; Mayer and Ellersieck, 1986;
Pisces															
Danio rerio	fertilised eggs	N	S	DNOC		tw	8.2	26	425	48 h	EC50	circulation	4.7	4	Schulte and Nagel, 1994
Danio rerio	fertilised eggs	N	S	DNOC		tw	8.2	26	425	48 h	EC50	mortality	5.2	5	Schulte and Nagel, 1994
Lepomis macrochirus	0.32-1.2 g	N	S	DNOC	≥ 80	rdw	6.5-7.9	21-23	32-48	96 h	LC50	mortality	0.23		Buccafusco *et al*., 1981
Lepomis macrochirus	1.0 g	N	S	DNOC	100	rdw	7.1	18	44	96 h	LC50	mortality	0.36		Mayer and Ellersieck, 1986
Oncorhynchus mykiss	1.2 g	N	S	DNOC	100	rdw	7.1	13	44	96 h	LC50	mortality	0.066		Mayer and Ellersieck, 1986
Pimephales promelas	30-35 d	Y	F	DNOC		lw		25±2	43.3-48.5	96 h	LC50	mortality	2.2		Phipps *et al*., 1981
Pimephales promelas	30-35 d	Y	F	DNOC		lw		25±2	43.3-48.5	96 h	LC50	mortality	1.9		Phipps *et al*., 1981
Pimephales promelas	30-35 d	Y	F	DNOC		lw		25±2	43.3-48.5	8 d	LC50	mortality	1.7		Phipps *et al*., 1981
Pimephales promelas	30-35 d	Y	F	DNOC		lw		25±2	43.3-48.5	8 d	LC50	mortality	1.3		Phipps *et al*., 1981
Pimephales promelas	31 d	Y	F	DNOC	rg	lw	7.47	25.2	48	96 h	LC50	mortality	1.95		Phipps *et al*., 1981
Pimephales promelas	29 d; 17 mm; 0.08 g	Y	F	DNOC	rg	lw	7.22	26.3	43	96 h	LC50	mortality	1.54		Geiger *et al*., 1983; Call *et al*., 1989
Pimephales promelas	26-34 d	Y	F	DNOC	>95	lw	7.8	25	45	96 h	LC50	mortality	2.7		Broderius *et al*., 1995

Notes

1 Maximally 0.75% DMSO used as solvent, shown to be not growth inhibiting to the test organism.
2 95% confidence interval LC50: 1.9-2.2.
3 According to OECD202, no further test conditions mentioned.
4 Endpoint: no circulation.
5 Endpoint: no heartbeat.

Table A5. 6. Acute toxicity of aniline to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Scenedesmus subspicatus		N	S			am	8	24		48 h	EC50	biomass	68		Kühn and Pattard, 1990, cited in EC, 2004
Scenedesmus subspicatus		N	S			am	8	24		48 h	EC50	growth rate	>750		Kühn and Pattard, 1990, cited in EC, 2004
Selenastrum capricornutum		N								96 h	EC50	biomass	19		Calamari *et al*., 1980, cited in EC, 2004
Crustacea															
Daphnia cucullata		N								48 h	EC50	immobilisation	0.68		Canton and Adema, 1978, cited in EC, 2004
Gammarus fasciatus		Y	F							96 h	EC50	immobilisation	2.3		Boeri, 1989, cited in EC, 2004
Daphnia magna		N								48 h	EC50	immobilisation	0.17		Gersich and Mayes, 1986, cited in EC, 2004
Daphnia magna		N	S			am	8		55	24 h	EC50	immobilisation	0.9		Kühn *et al*., 1988, cited in EC, 2004
Daphnia magna		N	S			am	8		55	48 h	EC50	immobilisation	0.3		Kühn *et al*., 1988, cited in EC, 2004
Daphnia magna		Y	R							48 h	EC50	immobilisation	0.16		Danish Environmental Protection Agency, 1996, cited in EC, 2004
Daphnia magna		Y	F							48 h	EC50	immobilisation	0.25		Holcombe *et al*., 1987, cited in EC, 2004
Daphnia pulex		N								48 h	EC50	immobilisation	0.1		Canton and Adema, 1978, cited in EC, 2004
Pisces															
Danio rerio		N	S							96 h	LC50	mortality	32	1	Wellens, 1982, cited in EC, 2004
Danio rerio		Y	R							96 h	LC50	mortality	57.5		Zok *et al*., 1991, cited in EC, 2004
Lepomis macrochirus		Y	F							96 h	LC50	mortality	49		Holcombe *et al*., 1987, cited in EC, 2004
Oncorhynchus mykiss		Y	F							96 h	LC50	mortality	36.2		Hodson et al., 1987, cited in EC, 2004
Oncorhynchus mykiss		Y	F							48 h	LC50	mortality	28.3		Abram and Sims, 1982, cited in EC, 2004
Oncorhynchus mykiss		Y	F							96 h	LC50	mortality	10.6		Abram and Sims, 1983, cited in EC, 2004
Pimephales promelas	larvae <24 h old	Y	F							96 h	LC50	mortality	68.6		Marchini et al., 1992, cited in EC, 2004
Pimephales promelas	larvae <24 h old	Y	F							168 h	LC50	mortality	60.2		Marchini et al., 1992, cited in EC, 2004
Pimephales promelas	larvae <24 h old	Y	F							168 h	NOEC	growth and mortality	15.7		Marchini et al., 1992, cited in EC, 2004

Notes

1 In the EU-RAR for aniline, a range of 32-33 $mg.L^{-1}$ is reported. 32 $mg.L^{-1}$ is selected.

Table A5. 7. Acute toxicity of epichlorohydrin to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Bacteria															
Escherichia coli	strain CC102	N	Sc		≥95	am	7.0	30		3 h	EC50	growth	316		Harder, 2002
Algae															
Pseudokirchneriella subcapitata		Y	Sc					23± 2		72 h	EC50	growth rate	24.2	1	INERIS, 2006
Crustacea															
Daphnia magna		Y	Sc		pa			19-22		48 h	EC50	immobility	11.94	2,3	INERIS, 2006
Pisces															
Carassius auratus	6.2 cm, 3.3 g	Y	Sc			tw	7.8 (6-8)	20	25	24 h	LC50	mortality	23	5	Bridie *et al*., 1979

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Oncorhynchus mykiss	2 yr old; cultured	N	Rc					16-21.5		24 h	LC50	mortality	27	4	Lysak and Marcinek, 1972
Poecilia reticulata	2-3 mo old	Y	Rc			am	6.8-7.1	21-23		14 d	LC50	mortality	0.65	7,8	Deneer *et al*., 1988
Rasbora heteromorpha	1.3-3 cm	N	IF		~100	rw	7.2	20	20	24 h	LC50	mortality	72	6	Alabaster, 1969
Rasbora heteromorpha	1.3-3 cm	N	IF		~100	rw	7.2	20	20	48 h	LC50	mortality	36	6	Alabaster, 1969
Rasbora heteromorpha	1.3-3 cm	N	IF		~100	rw	7.2	20	20	48 h	lethal treshold	mortality	18	6	Alabaster, 1969

Notes
1 OECD 201 with test water according to NF EN 28692 (May 1993).
2 NF EN ISO 6341.
3 Value is geomean of LC0 en LC100 (8.87 and 16.07 $mg.L^{-1}$ respectively; measured concentrations).
4 Test solutions renewed after 24 h; value is geomean of 48h-LC0 and 24h-LC100 (19 and 38 $mg.L^{-1}$ respectively).
5 No aeration, chemical analysis before and after testing.
6 Open test systems with semicontinuous renewal every 10 min. (100% in 50 minutes).
7 Daily renewal of test solutions.
8 >50% of concentration of tested substances found before renewal; nominal concentrations were used for determination of the effect value.

Table A5. 8. Acute toxicity of 1,2-dibromoethane to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Coelenterata															
Hydra oligactis	adults		R			am				48 h	LC50	mortality	70	4	Herring *et al*., 1988
Hydra oligactis	adults		R			am				72 h	LC50	mortality	50	4	Herring *et al*., 1988
Crustacea															
Daphnia magna	≤ 24 h	Y				dilute min. w		25±1	120	48 h	LC50	mortality	6.50	1,2,8	Kszos *et al.,* 2003
Cerodaphnia dubia	≤ 24 h	Y				dilute min. w		25±1	98	48 h	LC50	mortality	3.61	1,3,8	Kszos *et al.,* 2003
Pisces															
Pimephales promelas	5 d	Y	R			dilute min. w			98	96 h	LC50	mortality	4.30	1,8	Kszos *et al.,* 2003
Oryzias latipes	28-43 d old	Y	CF		>99.0	nw	7.88±0.18	25±1	38-52	96 h	LC50	mortality	32.1	1	Holcombe, 1994
Lepomis macrochirus	3-5 in.		S			nw	6.7	25±1	58	24 h	LC50	mortality	18	5,6,7,9	Davis and Hardcastle, 1959
Lepomis macrochirus	3-5 in.		S			nw	7.0	25±1	17	24 h	LC50	mortality	25	5,6,7,10	Davis and Hardcastle, 1959
Lepomis macrochirus	3-5 in.		S			nw	7.0	25±1	17	48 h	LC50	mortality	18	5,6,7,10	Davis and Hardcastle, 1959
Micropterus salmoides	3-5 in.		S			nw	6.7	25±1	58	24 h	LC50	mortality	15	5,6,7,9	Davis and Hardcastle, 1959
Micropterus salmoides	3-5 in.		S			nw	7.0	25±1	17	24 h	LC50	mortality	25	5,6,7,10	Davis and Hardcastle, 1959
Micropterus salmoides	3-5 in.		S			nw	7.0	25±1	17	48 h	LC50	mortality	15	5,6,7,10	Davis and Hardcastle, 1959

Notes
1 Closed system.
2 Five concentrations used.
3 Four concentrations used.
4 1,2-Dibromoethane dissolved in acetone.
5 TIm value is reported as LC50 value.
6 Hardness recalculated according to INS guidance.
7 Depth of aquarium ≥ 6 inch to limit escape of volatile components.
8 Hardness expressed as $mg.L^{-1}$.
9 Testwater is Ouachita River water.
10 Testwater is Bayou DeSiard water.

Table A5. 9. Acute toxicity of ethinylestradiol to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Desmodesmus subspicatus		N	S	EE2	>98	am				24 h	EC50	photosynthesis	12.4	1	Escher *et al*., 2005a,b
Scenedesmus subspicatus				EE2							EC50	biomass	0.84	2	Kopf, 1995
Cnidaria															
Hydra vulgaris		N	R	EE2		am	7.7	20±1	209	96 h	LC50	mortality	3.8	3	Pascoe *et al*., 2002
Crustacea															
Ceriodaphnia reticulata		N	S	EE2	>98%	nw		21-25		24 h	EC50	swim inhibition	1.814	4	Jaser *et al*., 2003
Sida crystallina		N	S	EE2	>98%	nw		21-25		24 h	EC50	swim inhibition	> 4.1	5	Jaser *et al*., 2003
Gammarus pulex	juv	N	R	EE2		dtw	6.9-7.3	16±1	87.9	10 d	LC50	mortality	0.84	6	Watts *et al*., 2001
Daphnia magna				EE2						24 h	EC50	immobilisation	5.7	7	Kopf, 1995
Insecta															
Chironomus riparius	1st & 2nd instar	N	R	EE2		am		±20		9 d	LC50	mortality	> 0.1	8	Meregalli and Ollevier, 2001
Pisces															
Danio rerio	adult			EE2	98					96 h	LC50	mortality	~ 1.7	9	Schäfers *et al*. 2006, Wenzel *et al*., 2001
Pimephales promelas	eggs	N	CF	EE2		dtw	6.8-7.8	24-26		20 d	LC50	mortality	> 1.0E-05	10	Van Aerle *et al*., 2002
Amphibia															
Rana pipiens	stage 26; 20-25 mg	N	R	EE2	tg	fw	6.5	18-20		14 d	LC50	mortality	0.89	11	Hogan *et al*., 2006
Rana pipiens	stage 26; 20-25 mg	N	R	EE2	tg	fw	6.5	18-20		14 d	LC50	mortality	0.82	12	Hogan *et al*., 2006
Rana sylvatica	stage 26; 20-25 mg	N	R	EE2	tg	fw	6.5	18-20		14 d	LC50	mortality	0.56	11	Hogan *et al*., 2006
Rana pipiens	stage 36; 1.0-1.2 mg	N	R	EE2	tg	fw	6.5	18-20		14 d	LC50	mortality	1.24	13	Hogan *et al*., 2006

Notes

1 EC50 was reported as log(1/EC50(M)) = 4.38. R^2 value for the concentration-effect curve was 0.639.
2 Test performed according to DIN 38412 Teil 9.
3 Concentrations were measured in the stock solutions, which confirmed the concentrations.
4 Concentrations measured in stock solutions.
5 Concentrations measured in stock solutions.
6 Median LC50 showed a decrease in time from approximately 8 $mg.L^{-1}$ after 24 h to approximately 2 $mg.L^{-1}$ after 120 h exposure (and 0.84 $mg.L^{-1}$ after 10 d)
7 Test performed according to OECD 202.
8 test vessels also contained 2 cm of Rhine sand.
9 Performed as a range-finding test for a chronic study. LC50 value reported as 'approximately'. Test conditions not reported, therefore test results will not be used in ERL derivation.
10 One concentration tested; fertilised eggs exposed for 0-20 days post hatch: no effect on survival hatchability, weight and length. Exposure during also 0-5, 5-10, 10-15 and 15-20 dph gave the same result.
11 Stage 26 corresponds with start of exogenous feeding; eight test concentrations, four replicates; carrier solvent: ethanol at 0.01%; (solvent) control mortality 0-3%.
12 Replicated experiment; stage 26 corresponds with start of exogenous feeding; eight test concentrations, four replicates; carrier solvent: ethanol at 0.01%; (solvent) control mortality 0-3%.
13 Stage 36 corresponds with start of hindlimb formation; eight test concentrations, four replicates; carrier solvent: ethanol at 0.01%; (solvent) control mortality 0-3%.

Table A5. 10. Acute toxicity of methyl bromide to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Chlorella pyrenoidosa	log-phase	Y	S		> 99.9	am	8.2±0.2	24±1	53.9	2 d	EC50	growth	5.0	1,3	Canton *et al*., 1980
Scenedesmus quadricauda	log-phase	Y	S		> 99.9	am	8.2±0.2	24±1	53.9	2 d	EC50	growth	3.2	1,3	Canton *et al*., 1980
Crustacea															
Daphnia magna	< 1 d	Y	S		> 99.9	am	7.7±0.5	19±1	209	2 d	LC50	mortality	2.2	1,3	Canton *et al*., 1980
Pisces															
Oryzias latipes	4-5 w	Y	R		> 99.9	am	7.7±0.5	23±2	209	4 d	LC50	mortality	0.7	1,2,3	Canton *et al*., 1980
Poecilia reticulata	3-4 w	Y	R		> 99.9	am	7.7±0.5	23±2	209	4 d	LC50	mortality	0.8	1,2,3	Canton *et al*., 1980

Notes
1 Closed system.
2 Renewal once per 2 days.
3 Hardness calculated based on Ca^{2+} and Mg^{2+} ions.

Table A5. 11. Acute toxicity of 6PPD to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Pseudokirchneriella subcapitata	20000 cells/ml	N	S	Santoflex 13		am	7.8-8.9	24±1		96 h	EC50	growth	0.668	1	EG&G Bionomics, 1978
Crustacea															
Daphnia magna		Y		6PPD						48 h	EC50	immobilisation	0.23	2	OECD, 2004
Pisces															
Oryzias latipes		Y		6PPD						96 h	LC50	mortality	0.028		OECD, 2004
Pimephales promelas	1.3 g; 40.1 mm	Y	CF	Santoflex 13		ww	7.7-7.9	22±2	250	96 h	LC50	mortality	0.45	3	Thompson *et al*., 1979

Notes
1 Species formerly known (and tested as) *Selenastrum capricornutum*. EC50 obtained by fitting a logistic dose-response relationship through original data. Acetone was used as a carrier (max. 0.05 ml per 125 ml flask); solvent control included which revealed no significant effect; test performed in triplicate; continuous illumination. Same result obtained for endpoint chlorphyll.
2 Original test not available (Full reference = 'Japanese Ministry of Environment'). The resulting concentration is reported as 'effective' as opposed to nominal.
3 LC50 derived from original study report. Acetone used as carrier, solvent control included; 16:8 h light:dark; test was prolonged to 28 d of which NOEC is reported under chronic tests. Same result also reported in BUA (1998).

Table A5. 12. Acute toxicity of 3,3'-dichlorobenzidine to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Bacteria															
Aeromonas hydrophila	aquatic sp.			DCB		nutrient broth	6.7	37		18 h	EC50	growth	> 100	1	Dutka and Kwan, 1981
Pseudomonas fluorescens				DCB		nutrient broth	6.7	37		18 h	EC50	growth	> 100		Dutka and Kwan, 1981
Spirillum volutans	aquatic sp.			DCB			6.7			2 h	EC90	motility	16	1	Dutka and Kwan, 1981
Algae															
Scenedesmus subspicatus		Y	S	DCB						72 h	EC50	growth rate	4.3		ECB, 2000a
Crustacea															
Daphnia magna		Y	S	DCB	83					48 h	EC50	immobility	2.47	2	ECB, 2000a
Daphnia magna	< 24 h	Y	R	DCB	98	fw	8.43	22.3	170	48 h	LC50	mortality	1.05		Brooke, 1991
Pisces															
Brachydanio rerio		Y	S	DCB	83					96 h	LC50	mortality	3.3	3	ECB, 2000a
Lepomis macrochirus		N	S	DCB						120 h	LC50	mortality	0.5		ECB, 2000a
Leuciscus idus		N	S	DCB						48 h	LC0	mortality	2.5	4	ECB, 2000a
Pimephales promelas	30 d, 20 mm, 0.103 g	Y	S	DCB	98	fw	7.24	22	52	96 h	LC50	mortality	2.08	5	Brooke, 1991
Pimephales promelas	30 d, 15 mm, 0.053 g	Y	S	DCB	98	fw	6.67	22.3	49	96 h	LC50	mortality	1.05	5	Brooke, 1991
Pimephales promelas	30 d, 20 mm, 0.103 g	N	CF	DCB	98	fw	6.83	21.5	51	96 h	LC50	mortality	1.77	6	Brooke, 1991

Notes

1 ECB (2000) mentions that at concentrations above the water solubility of DCB in water, precipipation at the bottom of the test vessel was observed; this is not mentioned in Dutka and Kwan (1981). However, 100 $mg.L^{-1}$ is far above the aqueous solubilty.
2 Tween 80 used as solvent; in the 5.6 to 32 $mg.L^{-1}$ treatments, turbidity was observed.
3 Tween 80 used as solvent; in the 10 $mg.L^{-1}$ treatment, compound precipitates were observed at the bottom of the test vessel.
4 Test criterion reported as 'SG = schälichkeitsgrenze', which is assumed to be the LC0 as the DIN 38412 guideline describes. Test was performed acc. to DIN 38412.
5 LC50 based on mean of all measured concentrations at 0, 24, 48, 72 and 96 hours.
6 LC50 based on actual concentrations.

Table A5. 13. Acute toxicity of p-tert-octylphenol to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Crustacea															
Acaria tonsa	10-12 d ad	Y	S	4-OP					18	48 h	LC50	mortality	0.42		Cited in Brooke *et al*., 2005
Mysidopsis bahia	<24 h		S	4-tert-OP			7.8-8.3	25	20	96 h	EC50	growth	0.053		Cited in Brooke *et al*., 2005
Pisces															
Cyprinodon variegatus	8-9 mo		R	4-tert-OP				27	14-16	72 h	LC50	mortality	0.72		Cited in Brooke *et al*., 2005
Fundulus heteroclitus	embryos	N	S	4-tert-OP					20	96 h	LC50	mortality	3.9		Cited in Brooke *et al*., 2005
Fundulus heteroclitus	new hatched larv.	N	S	4-tert-OP					20	96 h	LC50	mortality	0.29		Cited in Brooke *et al*., 2005
Fundulus heteroclitus	larvae, 2w	N	S	4-tert-OP					20	96 h	LC50	mortality	0.28		Cited in Brooke *et al*., 2005
Fundulus heteroclitus	larvae, 4w	N	S	4-tert-OP					20	96 h	LC50	mortality	0.34		Cited in Brooke *et al*., 2005

Table A5. 14. Acute toxicity of DNOC to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Bacteria															
Vibrio fischeri		N	S	DNOC		am				5 min	EC50	luminescence	6.6		Curtis *et al*., 1982
Vibrio fischeri		N	S	DNOC		am	5.0-8.0	15		5 min	EC50	luminescence	6.6		Kaiser and Ribo, 1998
Vibrio fischeri		N	S	DNOC		am	5.0-8.0	15		5 min	EC50	luminescence	6.3		Kaiser and Ribo, 1998
Vibrio fischeri		N	S	DNOC		am		15	20	30 min	EC50	luminescence	5.5		Gälli *et al*., 1994
Pisces															
Salmo salar	6.59 cm, 3.3 g	Y	R	DNOC				9.0		96 h	LT		0.18	1	Zitko *et al*., 1976

Notes

1 LT = lethal threshold = geometric mean of LOEC and LC50; result is calculated from a linear function of log K_{ow} obtained in this study.

Table A5. 15. Acute toxicity of epichlorohydrin to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Bacteria															
Vibrio fischeri		N	S			am		15	20	5 min	EC50	luminescence	2310		Benson and Stackhouse, 1986
Vibrio fischeri		N	S			am		15	20	10 min	EC50	luminescence	1160		Benson and Stackhouse, 1986
Vibrio fischeri		N	S			am		15	20	15 min	EC50	luminescence	670		Benson and Stackhouse, 1986

Table A5. 16. Acute toxicity of 1,2-dibromoethane to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Bacteria															
Vibrio fischeri			S	1,2-dibromoethane		am	6.1-7.2	15		5 m	EC50	luminescence	211.5	1	Blaha *et al.*, 1998
Algae															
Glenodinium halli			Sc	1,2-dibromoethane		rw		20 ± 2	25	7 d	EC50	growth inhibition	> 16	2,3	Erickson and Freeman, 1978
Isochrysis galbana			Sc	1,2-dibromoethane		rw		20 ± 2	25	7 d	EC50	growth inhibition	> 16	2,3	Erickson and Freeman, 1978
Skeletonema costatum			Sc	1,2-dibromoethane		rw		20 ± 2	25	7 d	EC50	growth inhibition	4	2,3	Erickson and Freeman, 1978
Thalassiosira pseudonana			Sc	1,2-dibromoethane		rw		20 ± 2	25	7 d	EC50	growth inhibition	> 16	2,3	Erickson and Freeman, 1978
Pisces															
Centropomus undecimalis	juv		S	1,2-dibromoethane		nw		22.9-25.9		48 h	LC50	mortality	6.2	4	Landau and Tucker, 1984
Centropomus undecimalis	developing emb/larv		S	1,2-dibromoethane		nw		25.5-29.9		36 h	LC50	mortality	0.04	4	Landau and Tucker, 1984
Cyprinodon variegatus	juv		S	1,2-dibromoethane		nw		22.9-25.9		48 h	LC50	mortality	4.8	4	Landau and Tucker, 1984

Notes
1 Species formerly known as *Photobacterium phosphoreum*; microtox test.
2 Closed system.
3 Test medium not further specified.
4 1,2-dibromoethane dissolved in acetone.

Table A5. 17. Acute toxicity of ethinylestradiol to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Crustacea															
Acartia tonsa	ad: 10-12d	N	S	EE2	>98	am		20	18	48 h	LC50	mortality	1.1	1	Andersen *et al*., 2001
Acartia tonsa	egg	N	R	EE2	>98	am		20	18	120 h	EC50	development	0.088	1	Andersen *et al*., 2001
Echinodermata															
Hemicentrotus pulcherrimus	egg/embryo	N	S	EE2		nsw		18		48 h	NOEC	development	0.092	2	Kiyomoto *et al*., 2006
Strongylocentrotus nudus	egg/embryo	N	S	EE2		nsw		18		48 h	NOEC	development	0.092	2	Kiyomoto *et al*., 2006
Strongylocentrotus nudus	egg/embryo	N	S	EE2		nsw		18		48 h	LC100	mortality	0.74	3	Kiyomoto *et al*. 2006

Notes
1 Salinity was reported for the culture medium only
2 Exposure from 0-48h after fertilisation (haf), 0-12 haf, 12-24 haf and 12-48 haf gave the same NOEC. Effects established visually (moprhology), no statistical confirmation.
3 Exposure from 0-48 haf and 0-12 haf caused complete mortality. Effects established visually (moprhology).

Table A5. 18. Acute toxicity of 3,3'-dichlorobenzidine to marine organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Bacteria															
Vibrio fischeri							6.7			15 min	EC50	luminescence	0.058	1	Dutka and Kwan, 1981
Crustacea															
Palaemonetes pugio	juv, <20 mm, from field	Y	R	DCB		fnw+salts	7.5	20	10	48 h	LC10	mortality	0.73	2	Burton and Fisher, 1990
Pisces															
Fundulus heteroclitus	juv, <23 d, from eggs	Y	R	DCB		fnw+salts	7.5	20	10	48 h	LC50	mortality	0.73	3	Burton and Fisher, 1990

Notes

1 *Vibrio fischeri* is formerly known as *Photobacterium phosphoreum*.
2 Result based on measured concentrations; filtered natural water with sea salts or deionised water was used as test/diluent water; 50% mortality was reached at the highest concentration tested, which was the solubility limit of DCB in this test.
3 Result based on measured concentrations; filtered natural water with sea salts or deionised water was used as test/diluent water; 50% mortality was reached at the highest concentration tested, which was the solubility limit of DCB in this test.

Table A5. 19. Chronic toxicity of pentaBDE to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Selenastrum capricornutum										96 h	NOEC	growth	0.0033-0.0065	1	Anonymus, 2005
Selenastrum capricornutum										24 h	EC10	growth	0.0027		Anonymus, 2005
Selenastrum capricornutum										24 h	EC10	biomass	0.0031		Anonymus, 2005
Crustacea															
Daphnia magna			F							4 d	EC50	mortality	0.017		Anonymus, 2005
Daphnia magna			F							7-21 d	EC50	mortality	0.014		Anonymus, 2005
Daphnia magna			F							14-21 d	EC50	reproduction	0.014		Anonymus, 2005
Daphnia magna			F							21 d	NOEC	growth	0.0053	2	Anonymus, 2005
Daphnia magna			F							21 d	LOEC	growth	0.0098	2	Anonymus, 2005
Pisces															
Oncorhynchus mykiss	embryos										NOEC	growth	0.0089	3	Anonymus, 2005
Oncorhynchus mykiss	embryos										NOEC	hatching, survival	≥ 0.016	3, 4	Anonymus, 2005

Notes
1 0.0033 used for SRC_{eco}-calculation.
2 Final endpoint; growth was measured as length.
3 E.l.s. test; administered compound: 0.23% triBDPE, 36.02% tetraBDPE, 55.1% pentaBDPE and 8.58% hexaBDPE
4 Endpoints valid for both embryos and larvae.

Table A5. 20. Chronic toxicity of p-tert-octylphenol to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Scenedesmus subspicatus		N	S	4-tert-OP						72 h	EC10	growth rate	0.3		Cited in Brooke *et al*., 2005
Selenastrum capricornutum		N	S	4-tert-OP	'high'			24-25		96 h	NOEC	growth rate	< 1.0		Cited in Brooke *et al*., 2005
Crustacea															
Daphnia magna										21 d	NOEC	reproduction	0.030	1	Cited in Brooke *et al*., 2005
Daphnia magna	ad + y	Y	F							21 d	NOEC	growth	0.037		Cited in Brooke *et al*., 2005
Daphnia magna	ad + y	Y	F							21 d	NOEC	reproduction	0.062		Cited in Brooke *et al*., 2005
Pisces															
Oncorhynchus mykiss	post hatch	F		4-tert-OP	99.22					60 d	NOEC	growth (fry)	0.0061	2	Cited in Brooke *et al*., 2005
Oncorhynchus mykiss	post hatch	F		4-OP				7-13	12.5	466 d	NOEC	growth (bw)	0.03	3	Cited in Brooke *et al*., 2005

Notes
1 Endpoint: adult mean length.
2 Endpoint: growth of fry.
3 Endpoint: body weight.

Table A5. 21. Chronic toxicity of benzo[b]fluoranthene to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$\mu g.L^{-1}$]	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		Y	S			am	-		215	72 h	EC10	growth	>1	1	Bisson *et al*., 2000, cited in EC, 2006
Crustacea															
Ceriodaphnia dubia	< 24 h	Y	R	-		nw	8.1±0.4		240±40	7 d	EC10	reproduction	>1.083	2	Bisson *et al*., 2000, cited in EC, 2006

Notes
1 6000-8000 lux.
2 Photoperiod 16:8 h light:dark at less than 500 lux.

Table A5. 22. Chronic toxicity of benzo[k]fluoranthene to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$\mu g.L^{-1}$]	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		Y	S			am	-		215	72 h	EC10	growth	>1	1	Bisson *et al*., 2000, cited in EC, 2006
Crustacea															
Ceriodaphnia dubia	< 24 h	Y	R		-	nw	8.1±0.4		240±40	7 d	EC10	reproduction	>1.08	2	Bisson *et al*., 2000, cited in EC, 2006
Pisces															
Brachydanio rerio	ELS	Y	IF			rw	7.8-8.2			28 d	NOEC	length, weight	<0.58		Hooftman and Evers-de Ruiter, 1992b, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF			rw	7.8-8.2			28 d	LC52	length, weight	0.58		Hooftman and Evers-de Ruiter, 1992b, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	NOEC	mortality	0.35	3	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	LC50	mortality	0.65	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	LC10	mortality	0.62	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	NOEC	length	<0.19	3	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	EC50	length	0.86	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	EC10	length	0.17	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	NOEC	weight	0.35	3	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	EC50	weight	0.50	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006
Brachydanio rerio	ELS	Y	IF		100	rw	7.9-8.2		206	42 d	EC10	weight	0.31	3,4	Hooftman and Evers-de Ruiter, 1992c, cited in EC, 2006

Notes
1 6000-8000 lux.
2 Photoperiod 16:8 h light:dark at less than 500 lux.
3 Actual conc. 36-109% of initial conc., average 72%.
4 Determined from presented data with log-logistic dose-response relationship.

Table A5. 23. Chronic toxicity of DNOC to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Bacteria															
Escherichia coli		N	S	DNOC		nw	7.5	27	214	48 h	NOEC	acid formation	100		Bringmann and Kühn, 1959
Escherichia coli		N	S	DNOC		nw	7.5-7.8	25	214	48 h	NOEC	glucose degradation	100		Bringmann and Kühn, 1960
Pseudomonas fluorescens		N	S	DNOC		am		22	81	7 h	NOEC	growth	10		Slooff and Canton, 1983
Pseudomonas fluorescens		N	S	DNOC		nw	7.5-7.8	25	214	48 h	NOEC	glucose degradation	30	1	Bringmann and Kühn, 1960
Pseudomonas fluorescens		N	S	DNOC		am	7.0	25	81	16 h	NOEC	glucose-assimilation	16		Bringmann, 1973
Pseudomonas putida		N	S	DNOC		am	7.0	25	81	16 h	NOEC	growth	16	2	Bringmann and Kühn, 1976, 1977, 1979, 1980
Cyanobacteria															
Microcystis aeruginosa		N	S	DNOC		am		23	22	96 h	NOEC	growth	3.2		Slooff and Canton, 1983
Microcystis aeruginosa		N	S	DNOC		am	7.0	27	55	8 d	NOEC	growth	0.15	2	Bringmann, 1975; Bringmann and Kühn, 1976, 1978a,b
Algae															
Chlorella vulgaris		N	S	DNOC	90	am	~ 8	20	24	96 h	NOEC	growth	100	3	Garten, 1990
Pseudokirchneriella subcapitata		N	S	DNOC	90	am	~ 8	20	24	96 h	NOEC	growth	1	3	Garten, 1990
Scenedesmus pannonicus		N	S	DNOC		am		23	51	96 h	NOEC	growth	10		Slooff and Canton, 1983
Scenedesmus quadricauda		N	S	DNOC		am	7.0		60	8 d	NOEC	growth	13	2	Bringmann and Kühn, 1978
Scenedesmus quadricauda		N	S	DNOC		nw	7.5	24	214	96 h	NOEC	growth	36		Bringmann and Kühn, 1959, 1960
Scenedesmus subspicatus		N	S	DNCO		am	8.0	24		48 h	EC10	growth	16		Kühn and Pattard, 1990
Protozoa															
Chilomonas paramaecium		N	S	DNOC		am	6.9	20	75	48 h	NOEC	growth	5.4	2	Bringmann *et al*., 1980
Entosiphon sulcatum		N	S	DNOC		am	6.9	25	75	72 h	NOEC	growth	5.4	2	Bringmann, 1978; Bringmann and Kühn, 1979, 1980
Microregma heterostoma		N	S	DNOC		am	7.5-7.8	27	214	28 h	NOEC	feed intake	30.0		Bringmann and Kühn, 1959
Uronema parduczi		N	S	DNOC		am	6.9	25	75	20 h	NOEC	growth	0.012	2	Bringmann and Kühn, 1980
Macrophyta															
Lemna minor		N	S	DNOC		am		25	255	7 d	NOEC	reproduction	0.32		Slooff and Canton, 1983
Coelenterata															
Hydra oligactis	budless	N	R	DNOC		am		18	200	21 d	NOEC	reproduction	0.32		Slooff and Canton, 1983
Rotifera															
Brachionus calyciflorus	newly hatched	N	S	DNOC	> 98	am	7.5	25	80-100	2 d	EC10	reproduction	0.55		Radix *et al*., 1999
Mollusca															
Lymnea stagnalis	5 mo. eggs	N	R	DNOC		am		20	200	40 d	NOEC	reproduction	0.032		Slooff and Canton, 1983
Lymnea stagnalis	5 mo. eggs	N	R	DNOC		am		20	200	40 d	NOEC	mortality	1.0		Slooff and Canton, 1983
Crustacea															
Daphnia magna	24 h	Y	R	DNOC		am	8.0	25	250	21 d	NOEC	reproduction	1.3	4	Kühn *et al*., 1989
Daphnia magna		N	R	DNOC	≥ 99					14 d	NOEC	reproduction	0.6		Luttik and Linders., 1990
Daphnia magna	<24 h	N	R	DNOC		am		19	200	21 d	NOEC	reproduction	1.0		Slooff and Canton, 1983
Daphnia magna	<24 h	N	R	DNOC		am		19	200	21 d	NOEC	mortality	1.0		Slooff and Canton, 1983
Daphnia magna	<24 h	N	R	DNOC		am	7.8-8.2	19	200	16 d	NOEC	growth	0.21		Deneer *et al*., 1988
Insecta															
Culex pipiens	1st instar	N	R	DNOC		am		27	200	25 d	NOEC	development	10.0		Slooff and Canton, 1983

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Culex pipiens	1st instar	N	R	DNOC		am		27	200	25 d	NOEC	mortality	10.0		Slooff and Canton, 1983
Pisces															
Pimephales promelas	eggs, <24 h	Y	CF	DNOC		lw	7.2	25.3	51	31-34d	NOEC	growth	0.18	5	Call *et al.*, 1989
Poecilia reticulata	3-4 w	N	R	DNOC		am		23	200	28 d	NOEC	mortality	1.0		Slooff and Canton, 1983
Poecilia reticulata	3-4 w	N	R	DNOC		am		23	200	28 d	NOEC	growth	1.0		Slooff and Canton, 1983
Oryzias latipes	eggs	N	R	DNOC		am		23	200	40 d	NOEC	mortality	0.1		Slooff and Canton, 1983
Oryzias latipes	eggs	N	R	DNOC		am		23	200	40 d	NOEC	growth	1.0		Slooff and Canton, 1983
Oryzias latipes	eggs	N	R	DNOC		am		23	200	40 d	NOEC	hatching	1.0		Slooff and Canton, 1983
Amphibia															
Xenopus laevis	<2 d	N	R	DNOC		am		20	200	100 d	NOEC	mortality	0.32		Slooff and Canton, 1983
Xenopus laevis	<2 d	N	R	DNOC		am		20	200	100 d	NOEC	growth	0.32		Slooff and Canton, 1983

Notes
1 Concentration of starting inhibition of glucose-assimilation.
2 TGK = NOEC
3 Growth based on chlorophyll-a concentration, measured at 24h and 96h.
4 Result based on nominal test concentrations.
5 Same result obtained for endpoints: mean length, mean wet weight, mean dry weight.

Table A5. 24. Chronic toxicity of aniline to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Bacteria															
Pseudomonas putida		N		S		am	7.0	25	81	16 h	TGK	biomass	130	1	Bringmann and Kühn, 1976, 1977, 1979, cited in EC, 2004
Cyanobacteria															
Microcystis aeruginosa		N		S		am	7.0	27	55	8 d	TGK	biomass	0.16	1	Bringmann, 1975, cited in EC, 2004
Algae															
Selenastrum capricornutum		N								4 d	NOEC	biomass	2		Calamari et al., 1980, cited in EC, 2004
Scenedesmus subspicatus		N		S		am	8	24		2 d	EbC10	biomass	22		Kühn and Pattard, 1990, cited in EC, 2004
Scenedesmus subspicatus		N		S		am	8	24		2 d	ErC10	growth rate	48		Kühn and Pattard, 1990, cited in EC, 2004
Protozoa															
Chilomonas paramaecium		N		S		am	6.9	20	75	48 h	TGK	biomass	250	1	Bringmann and Kühn, 1980a, cited in EC, 2004
Entosiphon sulcatum		N		S		am	6.9	25	75	72 h	TGK	biomass	24	1	Bringmann, 1978, cited in EC, 2004
Uronema parduczi		N		S		am	6.9	25	75	20 h	TGK	biomass	91	1	Bringmann and Kühn, 1980b, cited in EC, 2004
Crustacea															
Daphnia magna		Y		F				20		21 d	NOEC	reproduction	0.016	2	Hutton, 1989, cited in EC, 2004
Daphnia magna	<24 h, IRCHA	Y		R		am	8	25		21 d	NOEC		0.004	3	Kühn et al., 1988, cited in EC, 2004
Daphnia magna		Y		R				20		21 d	NOEC		0.024		Gerisch and Milazzo, 1988, cited in EC, 2004
Daphnia magna								24		14 d	NOEC		0.0208		Gerisch and Milazzo, 1988, cited in EC, 2004
Daphnia magna								24		14 d	NOEC		0.0102		Gerisch and Milazzo, 1988, cited in EC, 2004

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Pisces															
Pimephales promelas	embryos < 24 h	Y		F						32 d	NOEC	growth, mortality	0.39	4	Russom and Broderius, 1991, cited in EC, 2004

Notes
1 TGK=toxic threshold concentration. Can be considered as NOEC.
2 Testwater was unfiltered fish tank water.
3 Actual concentrations not determined in test vessels but in additional vessel without food and highest treatment. Nominal NOEC was corrected for recovery rate in this additional vessel.
4 ELS-study.

Table A5. 25. Chronic toxicity of epichlorohydrin to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Bacteria															
Pseudomonas putida		N	Sc			am	7.0	25	81	16 h	NOEC	growth inhibition	55	1	Bringmann and Kühn, 1976
Cyanobacteria															
Microcystis aeruginosa		N	Sc			am	7.0	27	55	8 d	NOEC	growth inhibition	6.0	1	Bringmann and Kühn, 1978
Protozoa															
Chilomonas paramaecium		N	Sc			am	6.9	20	75	48 h	NOEC	growth inhibition	29	1	Bringmann and Kühn, 1981
Entosiphon sulcatum		N	Sc			am	6.9	25	75	72 h	NOEC	growth inhibition	35	1	Bringmann and Kühn, 1980
Uronema parduczi		N	Sc			am	6.9	25	75	20 h	NOEC	growth inhibition	57	1	Bringmann and Kühn, 1981
Algae															
Pseudokirchneriella subcapitata		Y	Sc			am		23±2		72 h	EC10	growth rate inhibition	10.7	2	INERIS, 2006
Scenedesmus quadricauda		N	Sc			am	7.0	27	55	8 d	NOEC	growth inhibition	5.4	1	Bringmann and Kühn, 1980

Notes
1 NOEC set equal to TGK (Toxische Grenzkonzentration) or TT (toxicity threshold).
2 Species formerly known as *Selenastrum capricornutum*.

Table A5. 26. Chronic toxicity of 1,2-dibromoethane to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Pisces															
Oryzias latipes	larvae	Y	CF	1,2-dibromoethane	> 99.0	nw	7.9	25 ± 1	38.0-52.0	28 d	NOEC	growth	5.81	1	Holcombe, 1994

Notes
1 Closed system.

Table A5. 27. Chronic toxicity of ethinylestradiol to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Value [$ng.L^{-1}$]	Notes	Reference
Algae																
Scenedesmus subspicatus				EE2						72 h	EC10	biomass	0.054	54000	1	Kopf, 1995
Rotifera																
Brachionus calyciflorus	20 h old	N	S	EE2		am	7.5	25		72 h	NOEC	increase	5.1E-01	510000	2	Radix *et al*., 2002
Mollusca																
Marisa cornuarietis	adult	N	R	EE2		tw		22±1		6 m	LOEC	fecundity/mortality	1.0E-06	1	3	Schulte-Oehlman *et al*., 2004
Potamopyrgus antipodarum	adult	N	R	EE2	>98					9 w	NOEC	mortality	≥ 1.0E-04	≥ 100	4	Jobling *et al*., 2004
Potamopyrgus antipodarum	adult	N	R	EE2	>98					9 w	NOEC	growth	≥ 1.0E-04	≥ 100	4	Jobling *et al*., 2004
Potamopyrgus antipodarum	adult	N	R	EE2	>98					9 w	NOEC	embryo production	5.0E-06	5	5	Jobling *et al*., 2004
Crustacea																
Ceriodaphnia reticulata		N	S	EE2	>98	nw		21-25		21 d	EC50	mortality	> 0.500		6	Jaser *et al*., 2003
Sida crystallina		N	S	EE2	>98	nw		21-25		21 d	EC50	mortality	3.0E-01	300000	6	Jaser *et al*., 2003
Daphnia magna				EE2						21 d	NOEC	reproduction	10	10000000	7	Kopf, 1995
Insecta																
Chironomus riparius	eggs	Y	R	EE2		dw	6.9-7.3	20	87.9	see note	NOEC	weight (wet)	0.1	100000	8	Watts *et al*., 2003
Chironomus riparius	eggs	Y	R	EE2		dw	6.9-7.3	20	87.9	see note	NOEC	moulting delay	0.1	100000	8	Watts *et al*., 2003
Pisces																
Danio rerio	adult	Y	R	EE2	98	dtw		25-29		21 d	LOEC	fertility	5.0E-05	50	9	Van den Belt *et al*., 2001
Danio rerio	hatchling	N	R	EE2	98	tw	7.8	24.0±1.5	350	120 h	NOEC	hatching	1.0E-05	10		Versonnen and Janssen, 2004
Danio rerio	juvenile	N	R	EE2	98	tw	7.8	24.0±1.5	350	33 d	LC50	mortality	> 1.0E-04	> 100		Versonnen and Janssen, 2004
Danio rerio	adult	N	R	EE2	98	tw	7.8	24.0±1.5	350	14 d	LC50	mortality	> 1.0E-04	> 100		Versonnen and Janssen, 2004
Danio rerio	embryo	N	R	EE2	≥ 98	tw				3 m	NOEC	reproduction	1.0E-06	1.0	10	Van den Belt *et al*., 2003
Danio rerio	adult	Y	CF	EE2		rtw		28.5±0.5		210 d	NOEC	reproduction	5.0E-07	0.50	11	Nash *et al*., 2004
Danio rerio	eggs	Y	CF	EE2	98					life cycle	EC50	reproduction	1.1E-06	1.1	12	Segner *et al*., 2003
Danio rerio	eggs	Y	CF	EE2	98	tw	7.6-8.1	25.6±0.35		42 d	NOEC	reproduction	≥ 3.0E-06	≥ 3.0	13	Fenske *et al*., 2005
Danio rerio	eggs	Y	CF	EE2	98	tw	7.6-8.1	25.6±0.35		118 d	EC100	reproduction	3.0E-06	3.0	14	Fenske *et al*., 2005
Danio rerio	juvenile & adult			EE2	98					28 d	LC50	mortality	~ 0.0001	8	15	Wenzel *et al*., 2001
Danio rerio	eggs (F1)	Y	CF	EE2	98	tw	7.6-8.6	26.0±0.5		42-78 d	NOEC	mortality	1.1E-06	1.1	16	Wenzel *et al*., 2001
Danio rerio	eggs (F1)	Y	CF	EE2	98	tw	7.6-8.6	26.0±0.5		42-78 d	NOEC	growth (length)	3.0E-07	0.3	17	Wenzel *et al*., 2001
Danio rerio	eggs (F1)	Y	CF	EE2	98	tw	7.6-8.6	26.0±0.5		155 d	NOEC	egg production	3.0E-07	0.3	18	Wenzel *et al*., 2001
Danio rerio	eggs (F1)	Y	CF	EE2	98	tw	7.6-8.6	26.0±0.5		155 d	NOEC	no. of fertilised eggs	3.0E-07	0.3	19	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		35 d (174 d)	NOEC	mortality	≥ 2.0E-06	≥ 2.0	20	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		35 d (174 d)	NOEC	growth (length)	3.0E-07	0.3	20	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		75 d (214 d)	NOEC	growth (length)	3.0E-07	0.3	21	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		91-142 d (230-281 d)	NOEC	time to maturation	3.0E-07	0.3	22	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		141 d (280 d)	NOEC	egg production	3.0E-07	0.3	23	Wenzel *et al*., 2001
Danio rerio	eggs (F2)	Y	CF	EE2	98	tw	7.3-8.3	25.5±0.7		141 d (280 d)	NOEC	no. of fertilised eggs	3.0E-07	0.3	24	Wenzel *et al*., 2001
Danio rerio	2 d	N	R	EE2	98	dtw	7.0-7.6	27-29		60 d	NOEC	hatching	1.0E-06	1.0	25	Hill and Janz, 2003
Danio rerio	1 d post hatch	N	CF	EE2		fw	7-8	26±2		60 d	NOEC	intersex	< 1.0E-05	< 10	26	Örn *et al*., 2006
Danio rerio	1 d post hatch	N	CF	EE2		fw	7-8	26±2		60 d	LC100	mortality	1.0E-04	100	27	Örn *et al*., 2006
Oncorhynchus mykiss	adult	Y	CF	EE2		nw	8.10±0.3	12		2 m	LOEC	reproduction	1.0E-05	10	28	Schultz *et al*., 2003
Oryzias latipes	2-5d		R	EE2	98	dtw	7.4-7.8	25±2	80-100	± 4 m	NOEC	reproduction	2.0E-06	2.0	29	Balch *et al*., 2004
Oryzias latipes	adult	Y	CF	EE2	100	dtw		24±1		21 d	NOEC	fecundity	2.6E-04	261	30	Seki *et al*., 2002

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Value [$ng.L^{-1}$]	Notes	Reference
Oryzias latipes	hatchling	N	R	EE2	98	dtw	8.1	.		2 m	NOEC	egg production	1.0E-05	10		Scholz and Gutzeit, 2000
Oryzias latipes	adult	N	R	EE2		rss	6.6	25-27	82.5	14 d	NOEC	reproduction	≥ 5.0E-06	≥ 5.0	31	Tilton *et al*., 2005
Oryzias latipes	1 d post hatch	N	CF	EE2		fw	7-8	26±2		60 d	NOEC	intersex	1.0E-05	10	32	Örn *et al*., 2006
Pimephales promelas	embryo	Y	CF	EE2	100	dtw		25±1	≥ 40	305 d	NOEC	overall	1.0E-06	1.0	33	Lange *et al*., 2001
Pimephales promelas	eggs	Y	F	EE2	98	dtw	8.01±0.15	24.2±0.73		150 d	NOEC	fertility	1.6E-07	0.16	34	Parrot and Blunt, 2005
Pimephales promelas	adult	Y	CF	EE2	≥ 98	tw	7.5-8.2	15-25	213	21 d	NOEC	fertility	3.0E-06	3.0	35	Pawlowski *et al*., 2004
Pimephales promelas	adult	N	CF	EE2	≥ 98			25		21 d	NOEC	mortality	≥ 1.0E-04	≥ 100	4	Jobling *et al*., 2004
Pimephales promelas	adult	N	CF	EE2	≥ 98			25		21 d	NOEC	egg production	< 0.1E-07	< 0.1	36	Jobling *et al*., 2004
Poecilia reticulata	juvenile	Y	CF	EE2						108 d	NOEC	reproduction	4.4E-05	44	37	Kristensen *et al*., 2005
Poecilia reticulata	juv. <1 wk	Y	CF	EE2			7.0±0.3	22.8		108 d	NOEC	growth/coloration	4.4E-05	44	38	Nielsen and Baatrup, 2006
Amphibia																
Xenopus tropicalis	larvae	Y	R	EE2		dw+tw		26±0.2		~42 d	NOEC	survival, growth	≥ 1.9E-02	≥ 19000	39	Petterson *et al*., 2006
Xenopus tropicalis	juvenile, 1 mo	Y	R	EE2		dw+tw		26±0.2		~42 d	NOEC	sex ratio	< 3.0E-04	< 300	40	Petterson *et al*., 2006
Xenopus tropicalis	adult, 9 mo	Y	R	EE2		dw+tw		26±0.2		~42 d	NOEC	survival, growth	≥ 1.9E-02	≥ 19000	41	Petterson *et al*., 2006
Xenopus tropicalis	adult, 9 mo	Y	R	EE2		dw+tw		26±0.2		~42 d	NOEC	sex ratio	< 3.0E-04	< 300	41	Petterson *et al*., 2006

Notes

1 Test performed according to DIN 38412 Teil 9.
2 Stock solution concentrations were measured. NOEC was based on population increase rate and recalculated from a value of 1.72 $\mu M.L^{-1}$.
3 A NOEC could not be determined from this study. Endpoint was similar for mortality and fecundity. At 1 $ng.L^{-1}$ a statistically significant reduction in fecundity was observed, when compared to the control. Furthermore, mortality was also significantly higher and none of the snails survived the termination of the spawning season. This was also observed at the highest test concentration, but not at the intermediate concentrations: therefore, observed effects were not dose related.
4 Several test conditions not reported; no effects observed at highest test concentration, NOEC could thus not be established.
4 Several test conditions not reported; no effects observed at highest test concentration, NOEC could thus not be established.
5 Several test conditions not reported; a significant stimulation of embryo number was observed; since the consequences of the stimulation of embryo number at the population level was unknown (e.g. hatching or fitness of F1 animals) the NOEC for stimulation is not used for ERL derivation.
6 Concentrations measured in stock solutions. Endpoint based on mortality of the hatchlings.
7 Test performed according to OECD 202
8 Solvent: 0.5% ethanol; duration of exposure not reported, but all aquatic stages from egg to pupa were exposed.
9 Measured concentrations were 99±11% after renewals and 76±14% prior to next renewal. Results (male fertilisation) based on nominal concentrations.The LOEC was based on the % males with postexposure fertilisation >70% compared to a reference value, which was the % nonexposed males with fertilisation above 70% during preexposure breeding. This % dropped from 80-100% in the control to 0% at 5 $ng.L^{-1}$ although no significance indications were given. TSI (testis somatic index) showed a significant decrease at 10 $ng.L^{-1}$. Based on both results, the LOEC was determined to be 5 $ng.L^{-1}$.
10 Based on female reproductive succes.
11 Measured concentrations were 90-100% of nominal. Test concentrations: 0.5, 5 and 50 $ng.L^{-1}$. At the LOEC of 5 $ng.L^{-1}$, complete reproductive failure was observed (no viable eggs), which can be considerd as an EC100. Therefore, EE2 seems to have a steep dose-effect relationship on reproduction of the F1 in a multi-life-cycle-test with *Danio rerio*.
12 Reproduction measured as fertilisation succes; test lasted from egg to sexual maturation (approximately 90-120 d for *Danio rerio*); four concentrations tested. Test characteristics not reported.
13 Only one concentration tested; 5% effect: not significant; exposure 0-42 d post fertilisation; reproduction measured as fertlisation succes and fecudity; acetone used as carrier at 3 $nL.L^{-1}$, not tested in solvent control because of low level.
14 Only one concentration tested; spawning was completey inhibited; exposure was from 0 to 118 d post fertilisation; reproduction could not be measured because of complete inhibition; acetone used as carrier at 3 $nL.L^{-1}$, not tested in solvent control because of low level.
15 Performed as a range-finding test for a chronic study. LC50 value reported as 'approximately'. Test conditions not reported, therefore test results will not be used in ERL derivation.
16 Measured concentrations between 80-120% of nominal, but s.d. at lower concentrations relatively high (54-88%). Average measured concentrations were used. Endpoint is survival rate in the period between 42 and 78 d post fertilisation.
17 Measured concentrations between 80-120% of nominal, but s.d. at lower concentrations relatively high (54-88%). Average measured concentrations were used. Endpoint is pseudo specific growth determined as individual animal length at day 78 over mean length per vessel at 42 d post fertilisation.
18 Measured concentrations between 80-120% of nominal, but s.d. at lower concentrations relatively high (54-88%). Average measured concentrations were used. Endpoint is total no. of eggs per female per day.
19 Measured concentrations between 80-120% of nominal, but s.d. at lower concentrations relatively high (54-88%). Average measured concentrations were used. Endpoint is total no. of fertilised eggs per female per day. Same result was obtained for fertilisation capacity, which is percentage of fertilised eggs per female per test vessel per day.
20 Average measured concentrations were used; ELS test performed with eggs from animals that had been exposed for a complete life cycle (results from F1 generation by Schäfers *et al*. (2006) and Wenzel *et al*. (2001) also in this table).
21 Average measured concentrations were used; Test performed with eggs from animals that had been exposed for a complete life cycle (results from F1 generation by Schäfers *et al*. (2006) and Wenzel *et al*.(2001) also in this table).
22 Average measured concentrations were used; Test performed with eggs from animals that had been exposed for a complete life cycle (results from F1 generation by Schäfers *et al*. (2006) and Wenzel *et al*..(2001) also in this table). Endpoint measured as time to first spawning.
23 Average measured concentrations were used; test performed with eggs from animals that had been exposed for a complete life cycle (results from F1 generation by Schäfers *et al*. (2006) and Wenzel *et al*. (2001) also in this table); endpoint is total no. of eggs per female per day.
24 Average measured concentrations were used; test performed with eggs from animals that had been exposed for a complete life cycle (results from F1 generation by Schäfers *et al*. (2006) and Wenzel *et al*. (2001) also in this table). Endpoint is total no. of fertilised eggs per female per day. Same result was obtained for fertilisation capacity, which is percentage of fertilised eggs per female per test vessel per day.

25 A similar NOEC was observed for the percentage viable eggs.
26 All fish were female at end of exposure period, against 33%♂ and 67%♀ in control; solvent concentration not reported.
27 Solvent concentration not reported.
28 Measured concentrations were 60-90% at 1000 ng.L^{-1}, 120-140% at 100 ng.L^{-1} and 100-118% at 10 ng.L^{-1}. Results expressed on nominal basis.
29 Based on fertilisation succes of eggs produced by exposed females
30 Results are expressed based on average measured concentrations.
31 Test medium was reconstituted saline solution (1.6‰); NOEC can not be established since next higher test concentration showing significant effect is factor of 100 higher (500 ng.L^{-1}); reproduction measured as fecundity, %fertilisation, %hatching. Test can not be considered a full chronic test.
32 Only two concentrations tested; at 100 ng.L-1 treatment significant sex ratio shift (88%♀, 10%♂ and 2% intersex as opposed to control: 56%♂ and 54%♀). NOEC not used in ERL derivation since only 2 conc.'s were tested, difference between 'NOEC' and LOEC is a factor of 10; solvent concentration not reported.
33 Measured concentrations were 58-84% of nominal. Results were based on nominal concentrations.Due to the setup of the experiment, there was an unavoidable bias in starting the F1 early-life stage studies. Therefore, caution should be applied in interpreting the biological relevance of the statistical evaluation (NOEC < 0.2 ng.L^{-1}) relating to the F1 growth data. Taken as a whole, it was therefore considered that for all endpoints monitored, the overall biologically derived NOEC was 1 ng.L^{-1}.
34 Lowest test concentrations (0.32 and 0.96 ng.L^{-1}) were below the LOD (0.74-1.5 ng.L^{-1}) and were therefore reported nominally. The LOEC of 0.32 ng.L^{-1} showed approximately 15-18% effect. According to the TGD, in this case a NOEC can be calculated by dividing the LOEC by 2, resulting in a NOEC of 0.16 ng.L^{-1}
35 Temperature was gradually increased during experiment. Measured concentrations were 68-81% of nominal (at 1 and 10 ng.L^{-1}), no measured concentrations at NOEC were presented. Effects were expressed on nominal concentrations.
36 Several test conditions not reported; a significant stimulation egg production was observed at the lowest (and next higher) test concentration. Egg production decreased at higher concentrations until complete cessation at 100 ng.L-1.
37 NOEC based on the ability of exposed males to compete with control males for siring juveniles. The LOEC resulted into an almost total elimination of reproduction with only 1 of 17 exposed males fathering offspring in competition with unexposed males.
38 NOEC expresses both a significant stimulation of weight, sign. decrease of sex ratio as well as a sign. decrease in mating-enhancing orange coloration. Acetone used as solvent at 76 µl.L^{-1}.
39 Same result obtained for endpoint 'time to comlete metamorphosis'; ethanol used as solvent at 0.001%.
40 Animals exposed from 4-5 after hatching till methamorphosis completed (~42 d); after methamorphosis (ethanol used as solvent at 0.001%), then 1 month in clean water.
41 Animals exposed from 4-5 after hatching till methamorphosis completed (~42 d); after methamorphosis (ethanol used as solvent at 0.001%), then 9 months in clean water.

Table A5. 28. Chronic toxicity of methyl bromide to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$.L^{-1}]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Pisces															
Oryzias latipes	freshly fert eggs; < 6 h	Y	R	methyl bromide	>99.9	am				3 m	NOEC	growth	0.32	1,2	Wester *et al.,* 1988
Poecilia reticulata	3-4 w	Y	R	methyl bromide	>99.9	am				1 m	NOEC		0.1	1,3	Wester *et al.,* 1988

Notes
1 Closed system; DMSO used as solvent
2 actual conc. 59-89% (t=0 h) and 50-88% (t=48 h), not clear if the NOEC is based on nominal or actual concentrations.
3 actual conc. 75-78% (t=0 h) and 47- 56% (t=48 h), not clear if the NOEC is based on nominal or actual concentrations.

Table A5. 29. Chronic toxicity of 6PPD to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Pseudokirchneriella subcapitata	20000 cells/ml	N	S	Santoflex 13		am	7.8-8.9	24±1		96 h	EC10	growth	0.22	1	EG&G Bionomics, 1978
Pisces															
Pimephales promelas	1.3 g; 40.1 mm		IF	Santoflex 13		ww	7.7-7.9	22±2	250	28 d	NOEC	mortality	0.024	2	Thompson *et al*., 1979

Notes

1 Species formerly known (and tested as) *Selenastrum capricornutum*. EC10 obtained by fitting a logistic dose-response relationship through original data. Acetone was used as a carrier (max. 0.05 ml per 125 ml flask); solvent control included which revealed no significant effect; test performed in triplicate; continuous illumination. Same result obtained for endpoint chlorphyll.

2 NOEC derived from original study report. Result based on mean measured concentrations. Dissolved oxygen varied from 8.0 $mg.L^{-1}$ to 6.3 $mg.L^{-1}$.

Table A5. 30. Chronic toxicity of 3,3'-dichlorobenzidine to freshwater organisms.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3.L^{-1}$]	Exp. time	Criterion	Test endpoint	Value [$mg.L^{-1}$]	Notes	Reference
Algae															
Scenedesmus subspicatus		Y	S							72 h	NOEC	biomass	0.32		ECB, 2000a

Table A5. 31. Chronic toxicity of DNOC to marine organisms

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Bacteria															
Vibrio fischeri		N	S	DNOC	> 98	am	7.5	27	35	22 h	EC10	bioluminescence	0.039		Radix *et al*., 1999

Table A5. 32. Chronic toxicity of ethinylestradiol to marine organisms

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Crustacea															
Acartia tonsa	egg	N	R	EE2	>98	am	-	20	18	120 h	EC10	development	4.60E-02	1	Andersen *et al*., 2001
Tisbe battagliai	24 h old	N	R	EE2		nw	7.11-8.42	19.4-21.0	±35	21 d	NOEC	reproduction	≥0.1		Hutchinson *et al*., 1999
Tisbe battagliai	< 24 h	R	R	EE2		nw	7.11-8.42	20±1		21 d	NOEC	survival	≥0.1		Pounds *et al*. 2002
Tisbe battagliai	< 24 h	R	R	EE2		nw	7.11-8.42	20±1		21 d	NOEC	reproduction	≥0.1		Pounds *et al*. 2002
Pisces															
Cyprinodon variegatus	juvenile	Y	CF	EE2		nw	7.8-8.0	25.6-28.7	20-21	max. 59 d	NOEC	reproduction	2.00E-05	2	Zillioux *et al*., 2001
Cyprinodon variegatus	juvenile	Y	CF	EE2		nw	7.8-8.0	25.6-28.7	20-21	max. 59 d	NOEC	hatching	2.00E-05	2	Zillioux *et al*., 2001
Cyprinodon variegatus	juvenile	Y	CF	EE2		nw	7.8-8.0	25.6-28.7	20-21	max. 59 d	NOEC	survival	2.00E-04	2	Zillioux *et al*., 2001
Ptomatoschistus minutus	juvenile	N		EE2		nw	7.9-8.2	4.5-10.5		7.5 m	NOEC	growth	< 6.0E-06	3	Robinson *et al*., 2003

Notes
1 Salinity was reported for the culture medium only
2 At the lowest concentrations, stock solutions were analysed.
3 Only one (nominal) concentration tested, which had significant effect on male weight and length.

Table A5. 33.Toxicity of DNOC to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Bacteria															
Escherichia coli	ATCC 11775												101	1	
Crustacea															
Daphnia magna	<72 h							22		24 h	EC50	immobility	3.5-10		Devillers *et al*., 1985
Pisces															
Brachydanio rerio								22		24 h	LC50		1-3.5		Devillers *et al*., 1985
Cyprinus carpio	fertilised eggs	N	R	DNOC	tech	am (ISO)	6.9	24.5	250	13 d	NOEC	mortality, growth	<0.25		Ghillebaert *et al*., 1995
Cyprinus carpio	fertilised eggs	N	R	DNOC	tech	am (ISO)	6.9	24.5	250	13 d	NOEC	growth	≥ 0.25		Ghillebaert *et al*., 1995
Cyprinus carpio	fertilised eggs	N	R	DNOC	tech	am (ISO)	7.8	24.5	250	13 d	NOEC	mortality	1.0		Ghillebaert *et al*., 1995
Cyprinus carpio	fertilised eggs	N	R	DNOC	tech	am (ISO)	7.9	24.5	250	13 d	NOEC	growth	0.50		Ghillebaert *et al*., 1995
Cyprinus carpio	fertilised eggs	N	R	DNOC	tech	am (ISO)	9.0	24.5	250	13 d	NOEC	mortality, growth	≥ 2		Ghillebaert *et al*., 1995

Notes

1 No testmethods described.

Table A5. 34.Toxicity of aniline to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Bacteria															
activated sludge		N								0.167 h	EC50	respiration	2500		Mihara *et al*., 1991, cited in EC, 2004
activated sludge		N								2 h	EC50	nitrification	7		Bayer AG, 2000c, cited in EC, 2004
activated sludge		N								2 h	NOEC	nitrification	2		Bayer AG, 2000c, cited in EC, 2004
Pisces															
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	50	4 d	mortality	LC50	10.4	1,2	Birge *et al*., 1979, cited in EC, 2004
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	50	8 d	mortality	LC50	5.2	1,2	Birge *et al*., 1979, cited in EC, 2004
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	50	4 d	mortality	NOEC	0.045	1,2,3	Birge *et al*., 1979, cited in EC, 2004
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	200	4 d	mortality	LC50	8.4	1,2	Birge *et al*., 1979, cited in EC, 2004
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	200	8 d	mortality	LC50	4.4	1,2	Birge *et al*., 1979, cited in EC, 2004
Micropterus salmoides	eggs 1-2 h after spawning	Y	F				7.3-8.1	19-24	200	4 d	mortality	NOEC	0.051	1,2,3	Birge *et al*., 1979, cited in EC, 2004
Danio rerio	fertilised eggs, 1 d after spawning	Y	R				7.3-8.1	19-24	200	28 d	mortality, hatching, growth	NOEC	1.8	4	van Leeuwen *et al*., 1990, cited in EC, 2004
Danio rerio	fertilised eggs, 1 d after spawning	Y	R				7.3-8.1	19-24	200	28 d	mortality	NOLC	5.6	4,5	van Leeuwen *et al*., 1990, cited in EC, 2004

Notes

1 Embryo-larval test.

2 The effect concentrations for Micropterus salmoides were derived from a study of Birge et al. (1979). Effect concentrations found by birge and Black are usually very low compared to effect values found by other authors. Therefore, it was decided by the EU Member States not to use these data for M. salmoides if other valid fish ELS tests are vailable. Since this is the case, this study is rejected for PNECaqua derivation.

3 NOEC was rough estimate.

4 NOEC and NOLC based on nominal concentrations. Data were not used for RA, because not enough data on actual concentrations were supplied.

5 NOLC = no observed lethal concentration. In this semi-static study actual concentrations were analysed before and after renewal of the test solution. It was found that the measured aniline concentrations were far below the nominal concentrations.

Table A5. 35.Toxicity of epichlorohydrin to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Bacteria															
Salmonella typhimurium	strain TA104 *pr1*	N	Sc			am		37		4 h	NOEC	luminescence	≥ 512	9	Verschaeve *et al*., 1999
Algae															
Scenedesmus vacuolatus										2 h	EC50	photosystem II	1277		Niederer (2002) in Harder 2002
Crustacea															
Daphnia magna	<24 h, 0.315-0.630 mm	N	S			tw	7.6-7.7	20-22	286	24 h	EC50	immobility	30		Bringmann and Kühn, 1977
Daphnia magna	<24 h, 0.315-0.630 mm	N	S			tw	7.6-7.7	20-22	286	24 h	EC0/100	immobility	20 / 44		Bringmann and Kühn, 1977
Daphnia magna	<24 h, Strauss, IRCHA	N	S			am	8.0±0.2	20-22	250	24 h	EC50	immobility	40		Bringmann and Kühn, 1982
Daphnia magna	<24 h, Strauss, IRCHA	N	S			am	8.0±0.2	20-22	250	24 h	EC0	immobility	30		Bringmann and Kühn, 1982
Daphnia magna	<24 h, Strauss, IRCHA	N	S			am	8.0±0.2	20-22	250	24 h	EC 100	immobility	53		Bringmann and Kühn, 1982
Daphnia magna		N	S		rg	lw	7.7-8.3	20-22	157	24 h	LC50	mortality	33.4		Gersich *et al*., 1986
Daphnia magna		N	S		rg	lw	7.7-8.3	20-22	157	48 h	LC50	mortality	28.9		Gersich *et al*., 1986
Daphnia magna		N	S		rg	lw	7.7-8.3	20-22	157	48 h	LC50	mortality	22.6		Gersich *et al*., 1986
Daphnia magna		N	S		rg	lw	7.7-8.3	20-22	157	48 h	LC50	mortality	21.0		Gersich *et al*., 1986
Pisces															
Brachydanio rerio		N	S				7.5	20		96 h	LC50	mortality	30.5	1	Wellens, 1982
Brachydanio rerio		N	S				7.5	20		96 h	*LC0*		26	1	Wellens, 1982
Cyprinodon variegatus		N	S							96 h	LC50	mortality	11.8	5,6	Citation in Dawson *et al*., 1977
Lepomis macrochirus	33-75 mm	N	S			nw	7.6-7.9	23	55	24 h	LC50	mortality	ca. 42	2,3	Dawson *et al*, 1977
Lepomis macrochirus	33-75 mm	N	S			nw	7.6-7.9	23	55	48 h	LC50	mortality	37-42	2,3	Dawson *et al*, 1977
Lepomis macrochirus	33-75 mm	N	S			nw	7.6-7.9	23	55	72 h	LC50	mortality	37-42	2,3	Dawson *et al*, 1977
Lepomis macrochirus	33-75 mm	N	S			nw	7.6-7.9	23	55	96 h	LC50	mortality	35	2	Dawson *et al*, 1977
Leuciscus idus melanotus		N	S					20		48 h	LC50	mortality	24		Juhnke and Lüdemann, 1978
Leuciscus idus melanotus		N	S					20		48 h	LC0	mortality	12		Juhnke and Lüdemann, 1978
Leuciscus idus melanotus		N	S					20		48 h	LC100	mortality	35		Juhnke and Lüdemann, 1978
Menidia beryllina	40-100 mm, wild fish	N	S			rw	7.6-7.9	20		96 h	LC50	mortality	18	7,8	Dawson *et al*, 1975/77
Pimephales promelas	fry (10-15 d)	N	Sc		rg	lw	7.2-8.5	21-23	96-125	96 h	LC50	mortality	12.7	4	Mayes *et al*.,1983
Pimephales promelas	juvenile (30-35 d)	N	Sc		rg	lw	7.2-8.5	21-23	96-125	96 h	LC50	mortality	10.6	4	Mayes *et al*.,1983
Pimephales promelas	subadult (65-94 d)	N	Sc		rg	lw	7.2-8.5	21-23	96-125	96 h	LC50	mortality	13.2	4	Mayes *et al*.,1983

Notes

1 No aeration.
2 Test medium: potable well water; aeration after 24 h when required.
3 Estimated from data in the publication.
4 Oxygen saturation below 40% during test.
5 TLm is used as LC50.
6 Toxicity value is citation of information from Dow Chemical Company.
7 Salinity (specific gravity) 1.018.
8 Continuous aeration required.
9 Non-toxic in range 4-512 mg/l.

Table A5. 36.Toxicity of 1,2-dibromoethane to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Coelenterata															
Hydra oligactis	pre-exposed ad,14 d, 5 mg/L		R		am					24 h	mortality	LC50	294	1, 2	Herring *et al*., 1988
Hydra oligactis	pre-exposed ad,14 d, 5 mg/L		R		am					48 h	mortality	LC50	280	1, 2	Herring *et al*., 1988
Hydra oligactis	pre-exposed ad,14 d, 5 mg/L		R		am					72 h	mortality	LC50	217	1, 2	Herring *et al*., 1988

Notes

1 1,2-Dibromoethane dissolved in acetone.
2 Endpoints not used since adults were pre-exposed to 1, 2-dibromoethane and response data are not monotonically increasing with concentration.

Table A5. 37.Toxicity of methyl bromide to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Crustacea															
Daphnia magna	< 1 d	y	R		> 99.9	am	7.7±0.5	19±1	209	12 d	LC50	mortality	2.0	1	Canton *et al*., 1980
Pisces															
Cyprinus carpio	5-7 months	y	F			tw		22		2 d	LC50	mortality	17	2	Segers *et al*., 1984
Lepomis macrochirus	33-75 mm	y			tg	nw	7.6-7.9	23	55	96 h	LC50	mortality	12	3	Dawson *et al*, 1975/77
Menidia beryllina	40-100 mm		R	methyl bromide	tg	am	7.6 - 7.9	20	55	96 h	mortality	LC50	11	4	Dawson *et al*, 1975/77

Notes

1 Closed system, renewal once per 2-3 days; hardness calculated based on Ca2+ and Mg2+ ions; not acceptable, test duration 12 d.
2 Exposure 4 h, exp. 2 d, ethanol solvent; results not reliable: open system, exposure of 8-12 animals per concentration, after 4 h the concentration was measured and found to be 15%. Results were corrected for this measurement.
3 Open system, chemical loss by evaporation; concentration expressed as ml.l-1, recalculated assuming a density of 1.732 g/ml; not reliable: open system, no measurements.
4 Aerated, but not during the first 24 hours; concentration expressed as ml.l-1, recalculated assuming a density of 1.732 g/ml; not reliable: open system, no measurements.

Table A5. 38.Toxicity of 6PPD to aquatic organims: rejected data.

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Crustacea															
Daphnia magna	<24 h	N	SC	6PPD	>95	ww	7.6-8.3	22	218-274	48 h	EC50	immobilisation	>1.0	1	EPA, 2003; ECB, 2000
Daphnia magna	unfed	N	S	6PPD						48 h	EC50	immobilisation	0.79	2	ECB, 2000
Daphnia magna	fed	N	S	6PPD						48 h	EC50	immobilisation	1.3	3	ECB, 2000
Daphnia magna	<24 h	N	SC	6PPD	>95	ww	7.7-8.4	20	<250	48 h	EC50	immobilisation	0.82	4	EPA, 2003; ECB, 2000b
Daphnia magna	<24 h	N	SC	6PPD	>95	ww	7.6-8.3	22	218-274	48 h	EC50	immobilisation	0.51	5	EPA, 2003; ECB, 2000b

Species	Species properties	A	Test type	Test compound	Purity [%]	Test water	pH	T [°C]	Hardness [mg CaCO3/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Notes	Reference
Insecta															
Chironomus tentans	larvae, 10-14 d	N								48 h	EC50		0.99	6	ECB, 2000
Pisces															
Brachydanio rerio		N	S	6PPD	tech g					96 h	LC0	mortality	5	7	ECB, 2000
Lepomis macrochirus	3.8 cm	N	SC	6PPD	>95		6.7-7.2	22		24 h	LC50	mortality	0.65	8	EPA, 2003; ECB, 2000
Lepomis macrochirus	3.8 cm	N	SC	6 PPD	>95		6.7-7.2	22		48 h	LC50	mortality	0.45	8	EPA, 2003; ECB, 2000
Lepomis macrochirus	3.8 cm	N	SC	6 PPD	>95		6.7-7.2	22		96 h	LC50	mortality	0.40	9	EPA, 2003; ECB, 2000
Oncorhynchus mykiss	3.7 cm	N	SC	6 PPD	>95		6.8-7.0	12		24 h	LC50	mortality	0.28	10	EPA, 2003; ECB, 2000
Oncorhynchus mykiss	3.7 cm	N	SC	6 PPD	>95		6.8-7.0	12		48 h	LC50	mortality	0.18	10	EPA, 2003; ECB, 2000
Oncorhynchus mykiss	3.7 cm	N	SC	6 PPD	>95		6.8-7.0	12		96 h	LC50	mortality	0.14	11	EPA, 2003; ECB, 2000

Notes

1 Study summary from EPA report used as a source. Acetone used as carrier, solvent control included; Daphnids were exposed to test solution that had been spiked 24 h earlier with 6PPD; dissolved oxygen 6.4-8.5 mg/l.
2 Rejected since only a very short summary was available. Acetone used as carrier; confidence interval EC50=0.7-0.91 mg/l; Daphnids not fed, result for fed animals is also reported.
3 Rejected since only a very short summary was available. Acetone used as carrier; Daphnids fed during experiment, result for unfed animals is also reported.
4 Study summary from EPA report used as a source. Acetone used as carrier; solvent control included; 16:8 h light:dark; confidence interval EC50=0.71-0.94 mg/l.
5 Study summary from EPA report used as a source. Acetone used as carrier, solvent control included; Daphnids were exposed immediately after spiking the test solution with 6PPD; dissolved oxygen 6.4-8.5 mg/l.
6 Rejected since only a very short summary was available. Confidence interval EC50=0.6-1.25 mg/l.
7 LC100 was 100 mg/l. Powdered testsubstance was dispersed in water.
8 Rejected since dissolved oxygen was 2% of saturation at end of test. Acetone used as carrier; solvent control included.
9 Rejected since dissolved oxygen was 2% of saturation at end of test. Acetone used as carrier; solvent control included;confidence interval 96 hLC50=0.32-0.5 mg/l.
10 Rejected since dissolved oxygen was 26% of saturation at end of test. Acetone used as carrier; solvent control included.
11 Rejected since dissolved oxygen was 26% of saturation at end of test. Acetone used as carrier; solvent control included; confidence interval 96 h LC50=0.12-0.16 mg/l.

Appendix 6 Information on terrestrial toxicity

Contents

Legend

Species	organism used in the test.
Species properties	age, size, weight or life stage.
Soil type	USDA classification given, if available. Also: artificial soil or other description if necessary.
A	Y = test substance analyzed in test soil. N = test substance not analyzed in test soil. field empty = no data.
Purity	purity of the test compound: %active ingredient, ag = analytical grade, lg= laboratory grade, pa = pro analysis, rg = reagent grade, tg = technical grade.
pH	pH of the test soil.
o.m.	organic matter content of the soil, used to recalculated the test result in test soil to a value expressed in Dutch standard soil (10% o.m.).
Clay	%clay of the test soil.
T	temperature employed during the test.
Exp. time	Exposure time: h = hours, d = days, w = weeks, m = months, min. = minutes.
Criterion	EC50 = lowest short term test result showing 50% mortality; LC50 = lowest short term test result showing 50% effect; NOEC = no observed effect concentration; LOEC = lowest observed effect concentration; ECx = effect concentration causing x% effect.
Test endpoint	the biological parameter investigated.
Result test soil	the value expressing the result of the study (NOEC, EC10, etc.) as obtained in the experiment (or recalculated by the assessor, which is then mentioned in a note to the table), expressed in dry weight soil.
Result standard soil	the value expressing the result of the study (NOEC, EC10, etc.) as recalcuated to dry weight Dutch standard soil, containing 10% organic matter.
Notes	remarks to the summarised test result.
Reference	source of the study.

Table A6. 1. Acute toxicity of pentaBDE to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil mg.kg$_{dw}^{-1}$]	Notes	Reference
Annelida															
Eisenia fetida	artificial		Y		6.6-7.6 => 7.7-8.7	10	20	20	14 d	NOEC	mortality	≥ 456	≥ 456	1	EC, 2001

Notes
1 Composition of test compound was 0.23%triBDPE, 36.02% tetraBDPE, 55.1% pentaBDPE and 8.58% hexaBDPE; same result obtained for the endpoint growth (weight); result expressed as mean actual concentration.

Table A6. 2. Acute toxicity of DNOC to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Oligochaeta															
Allolobophora chlorotica	ad, 0.24-0.3 g	sand	N		~7	2	5	15	7 d	LC50	mortality	13	65		Fayolle, 1979
Eisenia fetida	ad, > 2 mo	artificial soil	N	WP	7	10.5	5	22	28 d	LC50	mortality	21	20	1	Heimbach, 1984

Notes
1 Test compound added as wettable powder, containing 40% active ingredient; LC50 expressed as a.i.

Table A6. 3. Acute toxicity of aniline to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Macrophyta															
Latuca sativa			Y			1.8			14 d	EC50	growth	33	183.3	1	Hulzebos *et al*., 1993, cited in EC, 2004
Latuca sativa			Y			1.4			14 d	EC50	growth	56	400.0	1	Hulzebos *et al*., 1993, cited in EC, 2004

Notes
1 Effect concentrations are based on nominal concentrations. Actual concentrations dropped to <30% after 14 days.

Table A6. 4. Acute toxicity of methy lbromide to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Macrophyta															
Abutilon theophrasti	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	8.3	8.6		Zhang *et al.*, 1997
Amaranthus retroflexus	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	2.4	2.5		Zhang *et al.*, 1997
Brassica kaber	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	7.9	8.2		Zhang *et al.*, 1997
Chenopodium album	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	4.7	4.9		Zhang *et al.*, 1997
Cyperus rotundus	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	11.6	12.1		Zhang *et al.*, 1997
Cyperus esculentus	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	6.4	6.7		Zhang *et al.*, 1997
Lolium multiflorum	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	6.8	7.1		Zhang *et al.*, 1997
Portulaca oleracea	seeds/tubers	loamy sand			6.2	9.6	4	25	2 d	EC50	germination	15.3	15.9		Zhang *et al.*, 1997

Table A6. 5. Chronic toxicity of pentaBDE to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Macrophyta															
Allium cepa	seed	artifical,sand	Y		7.5	2.9	8		21 d	NOEC	emergence	≥ 1000	≥ 3448	1,2	EC, 2001
Cucumis sativa	seed	artifical,sand	Y		7.5	2.9	8		21 d	NOEC	emergence	≥ 1000	≥ 3448	1,2	EC, 2001
Glycine max	seed	artifical,sand	Y		7.5	2.9	8		21 d	NOEC	emergence	≥ 1000	≥ 3448	1,2	EC, 2001
Lolium perenne	seed	artifical,sand	Y		7.5	2.9	8		21 d	NOEC	emergence	≥ 1000	≥ 3448	1,2	EC, 2001
Lycopersicon esculentum	seed	artifical,sand	Y		7.5	2.9	8		21 d	NOEC	emergence	125	431	1,2	EC, 2001
Zea mays	seed	artifical,sand	Y		7.5	2.9	8		21 d	EC5	emergence	16	55.2	1,3	EC, 2001

Notes
1 Same result was found for endpoints growth and condition; composition of test compound was 0.23%triBDPE, 36.02% tetraBDPE, 55.1% pentaBDPE and 8.58% hexaBDPE.
2 NOEC based on nominal concentrations.
3 EC5 is considered as NOEC in the EU-RAR, NOEC on basis of nominal concentrations.

Table A6. 6. Chronic toxicity of benzo[b]fluoranthene to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Collembola															
Folsomia fimetaria	23-26 d	sandy loam			6.2	2.7	13	20	21 d	LC50	mortality	> 360	> 1333	1	Sverdrup *et al.*, 2002, cited in EC, 2006
Folsomia fimetaria	23-26 d	sandy loam			6.2	2.7	13	20	21 d	EC10	reproduction	> 360	> 1333	1	Sverdrup *et al.*, 2002, cited in EC, 2006

Notes
1 12:12 h photoperiod under lighting of about 400-888 lux; values given are based on initial measured concentrations.

Table A6. 7. Chronic toxicity of benzo[k]fluoranthene to soil organisms.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [[mg.kg$_{dw}^{-1}$]	Notes	Reference
Collembola															
Folsomia fimetaria	23-26 d	sandy loam			6.2	2.7	13	20	21 d	LC50	mortality	> 560	> 2074	1	Sverdrup *et al.*, 2002, cited in EC, 2006
Folsomia fimetaria	23-26 d	sandy loam			6.2	2.7	13	20	21 d	EC10	reproduction	>.560	> 2074	1	Sverdrup *et al.*, 2002, cited in EC, 2006
Folsomia candida	10-12 d	artif. soil				10	20		28 d	NOEC	reproduction	≥ 180	≥ 180	2	Bowmer *et al.*, 1993, cited in EC, 2006

Notes
1 12:12 h Photoperiod under lighting of about 400-888 lux; values given are based on initial measured concentrations.
2 Endpoint (nr. of cocoons); 82-93% of nominal concentration; 37% reduction but not significant compared with control.

Table A6. 8. Chronic toxicity of 1,2-dibromoethane to soil organisms.

Process/Activity	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	Temp [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Fungi															
Verticillium dahliae	< 100 µM diameter	light medium clay			6.4	5.53		24	16 d	EC10	germination	1.82	3.29	1	Ben-Yephet *et al.*, 1981

Notes
1 Sealed system; endpoint is germination of microsclerotia.

Table A6. 9. Toxicity of pentaBDE to soil microbial processes and/or enzymatic reactions.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Microbial processes															
Nitrification		sandy loam	N		6.8	1.7		20	28 d	NOEC	nitrate production	> 1	> 5.9	1	EC, 2001

Notes
1 Composition of test compound was 0.23%triBDPE, 36.02% tetraBDPE, 55.1% pentaBDPE and 8.58% hexaBDPE.

Table A6. 10. Toxicity of DNOC to soil microbial processes and/or enzymatic reactions.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Microbial processes															
glucose respiration		loam	N	formulation	6.7	1.5	12	20	4 w	NOEC	CO_2 formation	< 4.9	< 31.9	1	Malkomes, 1999
glucose respiration		loam	N	formulation	7.4	2.9	22	20	12 w	NOEC	CO_2 formation	4.9	16.9	2	Malkomes, 1999
glucose respiration		loam	N	formulation	6.8	1.2	10.5	20	2 w	NOEC	CO_2 formation	< 4.9	< 42.2	3	Malkomes, 1990
glucose respiration		loam	N	formulation	7.2	1.7	23.1	20	12 w	NOEC	CO_2 formation	< 4.9	< 29.7	3	Malkomes, 1990
glucose respiration		loam	N	formulation	6.8	1.2	10.5	20	16 w	NOEC	CO_2 formation	< 4.9	< 42.2	4	Malkomes, 1990
glucose respiration		loam	N	formulation	7.2	1.7	23.1	20	16 w	NOEC	CO_2 formation	4.9	29.7	4	Malkomes, 1990
Enzyme activity															
dehydrogenase		loam	N	formulation	6.7	1.5	12	20	4 w	NOEC	inhibition	< 4.9	< 31.9	1	Malkomes, 1999
dehydrogenase		loam	N	formulation	7.4	2.9	22	20	12 w	NOEC	inhibition	4.9	16.9	1	Malkomes, 1999
dehydrogenase		loam	N	formulation	6.8	1.2	10.5	20	16 w	NOEC	inhibition	< 4.9	< 42.2	5	Malkomes, 1990
dehydrogenase		loam	N	formulation	7.2	1.7	23.1	20	16 w	NOEC	inhibition	< 4.9	< 29.7	6	Malkomes, 1990
dehydrogenase		loam	N	formulation	6.8	1.2	10.5	20	16 w	NOEC	inhibition	< 4.9	< 42.2	7	Malkomes, 1990
dehydrogenase		loam	N	formulation	7.2	1.7	23.1	20	12 w	NOEC	inhibition	< 4.9	< 29.7	7	Malkomes, 1990

Notes

1 A formulation ('Etzel' - water soluble concentrate) containing 556 g.L^{-1} DNOC was tested in two concentrations plus a control; soil amended with lucerne meal. pH = pH KCl.
2 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1} DNOC was tested in two concentrations plus a control; soil amended with lucerne meal. Same result obtained at 4 and 8 weeks of incubation. pH = pH KCl
3 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1} DNOC was tested in two concentrations plus a control; soil not amended with lucerne meal. Same result obtained at 1 and 2 weeks of incubation. pH = pH KCl.
4 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1} DNOC was tested in two concentrations plus a control; soil amended with lucerne meal. Same result obtained at 2, 4, 8 and 12 weeks of incubation. pH = pH KCl.
5 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1}l DNOC was tested in two concentrations plus a control; soil not amended with lucerne meal. Same result obtained at 1, 2, 4 and 8 weeks of incubation. pH = pH KCl.
6 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1} DNOC was tested in two concentrations plus a control; soil not amended with lucerne meal. Same result obtained at 1 and 2 weeks of incubation. pH = pH KCl.
7 A formulation ('Etzel' - water soluble concentrate) containing 556 g L^{-1} DNOC was tested in two concentrations plus a control; soil amended with lucerne meal. Same result obtained at 1, 2, 4 and 8 weeks of incubation. pH = pH KCl.

Table A6. 11. Toxicity of DNOC to soil organisms: rejected studies.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Macrophyta															
Raphanus sativus	germinated plants	artificial soil	N	90	5.3				28 d	NOEC	growth	1			Garten, 1990
Hordeum vulgare	germinated plants	artificial soil	N	90	5.3				28 d	NOEC	growth	10			Garten, 1990

Table A6. 12. Toxicity of 1,2-dibromoethane to soil organisms: rejected studies.

Process/Activity	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	Temp [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Nematoda															
Heterodera schachtii	sandy loam soil						11	21 - 22	3 d	LC50	mortality	215		2, 3	Abdella and Lear, 1975
Meloidogyne incognita	sandy loam soil						11	21 - 22	3 d	LC50	mortality	163		2, 3	Abdella and Lear, 1975
Paratylenchus sp.	sandy loam soil						11	21 - 22	3 d	LC50	mortality	461		2, 3	Abdella and Lear, 1975
Xiphinema index	sandy loam soil						11	22	3 d	LC50	mortality	115		2, 3	Abdella and Lear, 1975
Xiphinema index	sandy loam soil						11	15	3 d	LC50	mortality	893		2, 3	Abdella and Lear, 1975
Xiphinema index	sandy loam soil						11	20	3 d	LC50	mortality	143		2, 3	Abdella and Lear, 1975
Xiphinema index	sandy loam soil						11	30	3 d	LC50	mortality	106		2, 3	Abdella and Lear, 1975

Notes
1 Sealed bottles, equilibrium concentration in the liquid phase was used as the IC50.
2 Unknown according to which soil classification.
3 Particle size not reported.

Table A6. 13. Toxicity of methyl bromide to soil organisms: rejected studies.

Species	Species properties (age, sex)	Soil type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test soil [mg.kg$_{dw}^{-1}$]	Result stand. soil [mg.kg$_{dw}^{-1}$]	Notes	Reference
Bacteria															
methanogenic bacteria		laboratory culture, 900 mg L^{-1} VSS			7			35	48 h	gas production	IC50	3.9		1	Blum and Speece, 1991

Notes
1 Sealed bottles, equilibrium concentration in the liquid phase was used as the IC50; results can not be used for MPC derivation, test performed in liquid media.

Appendix 7 Information on sediment toxicity

Contents

Legend

Species	organism used in the test.
Species properties	age, size, weight or life stage.
Sediment type	description of sediment, e.g. artificial, muddy, sandy, loamy, anaerobic, etc.
A	Y = test substance analyzed in test. N = test substance not analyzed in test. field empty = no data.
Purity	purity of the test compound: %active ingredient, ag = analytical grade, lg= laboratory grade, pa = pro analysis, rg = reagent grade, tg = technical grade.
pH	pH in the test system, usually of the overlying water.
o.m.	organic matter content of the sediment, used to recalculated the test result in test sediment to a value expressed in Dutch standard sediment (10% o.m.).
Clay	%clay of the test sediment.
T	temperature employed during the test.
Exp. time	Exposure time: h = hours, d = days, w = weeks, m = months, min. = minutes.
Criterion	EC50 = lowest short term test result showing 50% mortality; LC50 = lowest short term test result showing 50% effect; NOEC = no observed effect concentration; LOEC = lowest observed effect concentration; ECx = effect concentration causing x% effect.
Test endpoint	the biological parameter investigated.
Result test sediment	the value expressing the result of the study (NOEC, EC10, etc.) as obtained in the experiment (or recalculated by the assessor, which is then mentioned in a note to the table), expressed in dry weight sediment.
Result standard sediment	the value expressing the result of the study (NOEC, EC10, etc.) as recalcuated to dry weight Dutch standard sediment, containing 10% organic matter.
Notes	remarks to the summarised test result.
Reference	source of the study.

Table A7. 1. Chronic toxicity data of pentaBDE to sediment dwelling organisms.

Species	Species properties (age, sex)	Sediment type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test sediment [mg.kg$_{dw}^{-1}$]	Result std. sediment [mg.kg$_{dw}^{-1}$]	Notes	Reference
Annelida															
Lumbriculus variegatus	adults	artificial	Y		8	<2	0.11	23	28	NOEC	survival, reproduction	3.1	18.2		EC, 2001
Lumbriculus variegatus	adults	artificial	Y		8	<2	0.11	23	28	LOEC	survival, reproduction	6.3	37.0		EC, 2001
Insecta															
Hyallella azteca										NOEC		6.3	37.0		EC, 2001
Chironomus riparius			Y							NOEC		16	94.1		EC, 2001
Chironomus riparius			Y							LOEC		28	164.6		EC, 2001

Table A7. 2. Chronic toxicity data of benzo[b]fluoranthene to sediment dwelling organisms.

Species	Species properties (age, sex)	Sediment type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test sediment [mg.kg$_{dw}^{-1}$]	Result std. sediment [mg.kg$_{dw}^{-1}$]	Notes	Reference
Crustacea															
Rhepoxynius abronius		sediment				4.4		15	10 d	LC50	mortality	> 46	> 180	1,3	Boese *et al*., 1998, cited in EC, 2006
Rhepoxynius abronius		sediment				4.4		15	10 d	EC50	reburial	> 46	> 180	1,3	Boese *et al*., 1998, cited in EC, 2006
Rhepoxynius abronius		sediment				4.4		15	10 d	LC50	mortality	> 46	> 180	2,3	Boese *et al*., 1998, cited in EC, 2006
Rhepoxynius abronius		sediment				4.4		15	10 d	EC50	reburial	> 46	> 180	2,3	Boese *et al*., 1998, cited in EC, 2006

Notes
1 Sediment (muddy sand) with overlying seawater (28 ‰) exposure for 10 days; 1 h reburial in control sediment.
2 1 h UV radiation after 10 days exposure and 1 h reburial: UV-A (321-400 nm) 315±36 µW.cm^{-2} and UV-B (280-320 nm) 128±12 µW cm^{-2} and visible light (401-700 nm) 3400±278 µW cm^{-2}; after irradiation again 1 h reburial.
3 L(E)C50 values given as µmol.g^{-1} OC (2.58%) is converted to mg.kg^{-1} sediment.

Table A7. 3. Chronic toxicity data of benzo[k]fluoranthene to sediment dwelling organisms.

Species	Species properties (age, sex)	Sediment type	A	Purity [%]	pH	o.m. [%]	Clay [%]	T [°C]	Exp. time	Criterion	Test endpoint	Result test sediment [mg.kg$_{dw}^{-1}$]	Result std. sediment [mg.kg$_{dw}^{-1}$]	Notes	Reference
Crustacea															
Daphnia magna	<24 h	sediment	Y			3.4	30	20	24 h	EC5	immobility	300	1500	1	Verrhiest *et al*., 2001, cited in EC, 2006
Daphnia magna	<24 h	sediment	Y			3.4	30	20	48 h	EC45	immobility	300	1500	1	Verrhiest *et al*., 2001, cited in EC, 2006
Hyalella azteca	2-3 w	sediment	Y			3.4	30	20	14 d	NOEC	mortality/growth	≥ 300	≥ 1500	1	Verrhiest *et al*., 2001, cited in EC, 2006
Insecta															
Chironomus riparius	larvae, 48 h	sediment	Y			3.4	30	20	10 d	NOEC	mortality/growth	≥ 300	≥ 1500	1	Verrhiest *et al*., 2001, cited in EC, 2006

Notes
1 Based on nominal concentrations; exposure under white light (2500 lux, 74-92 µW cm^{-2}), 16 h light/8 h dark.

Appendix 8 Information on air toxicity

Contents

Legend

Species	organism used in the test.
Species properties	age, size, weight or life stage.
A	Y = test substance analyzed in test. N = test substance not analyzed in test. field empty = no data.
Purity	purity of the test compound: %active ingredient, ag = analytical grade, lg= laboratory grade, pa = pro analysis, rg = reagent grade, tg = technical grade.
T	temperature employed during the test.
Exp. time	Exposure time: h = hours, d = days, w = weeks, m = months, min. = minutes.
Criterion	EC50 = lowest short term test result showing 50% mortality; LC50 = lowest short term test result showing 50% effect; NOEC = no observed effect concentration; LOEC = lowest observed effect concentration; ECx = effect concentration causing x% effect.
Test endpoint	the biological parameter investigated.
Value	test result; > and ≥ symbols = no effect observed at highest test concentration.
Notes	remarks to the summarised test result.
Reference	source of the study.

Table A8. 1. Acute toxicity data of aniline to organisms exposed via air.

Species	Species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Macrophyta										
Avena sativa	seeds and germ. plants	Y			14 d	EC50	changes	> 0.001	1,2	BASF, 2002 in EC, 2004
Avena sativa	seeds and germ. plants	Y			14 d	NOEC	length, weight, changes	0.001	1,3	BASF, 2002 in EC, 2004
Brassica pekinensis	seeds and germ. plants	Y			14 d	EC50	changes	> 0.001	1,2	BASF, 2002 in EC, 2004
Brassica pekinensis	seeds and germ. plants	Y			14 d	NOEC	length, weight, changes	0.0003	1,3	BASF, 2002 in EC, 2004
Abies grandis	seeds and germ. plants	Y			14 d	EC50	changes	> 0.001	1,2	BASF, 2002 in EC, 2004
Abies grandis	seeds and germ. plants	Y			14 d	NOEC	changes	> 0.001	1,2	BASF, 2002 in EC, 2004

Notes
1. Tested were seeds and germinated plants (1 year old) were acclimisted for 8 days before being exposed to three concentrations + control. Concentrations were analysed, test results based on nominal concentrations as these were close to actual.
2. Endpoint 'changes': microscopic and macroscopic changes observed in plants.
3. Endpoints 'length' and 'weight' were determined as growth, wet and dry weight, respectively.

Table A8. 2. Acute toxicity data of 1,2-dibromoethane to organisms exposed via air.

Species	Species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Insecta										
Acanthoscelides obtectus	1-2 wks old			26	2 h	LC50	mortality	21.0	1, 2, 3	Lindgren *et al.*, 1954
Acanthoscelides obtectus	1-2 wks old			26	6 h	LC50	mortality	10.2	1, 2, 3	Lindgren *et al.*, 1954
Callosobruchus chinensis	adult 1 d				24 h	LC50	mortality	5.649	1	Adu *et al.*, 1985
Callosobruchus chinensis	2-3 days old pupae				24 h	LC50	mortality	1.047	1	Adu *et al.*, 1985
Callosobruchus chinensis	larvae third instar				24 h	LC50	mortality	0.499	1	Adu *et al.*, 1985
Callosobruchus chinensis	eggs 1d				24 h	LC50	mortality	0.243	1	Adu *et al.*, 1985
Oryzaephilus surinamensis	2-6 wks			26	2 h	LC50	mortality	1.8	1, 2, 3	Lindgren *et al.*, 1954
Oryzaephilus surinamensis	2-6 wks			26	6 h	LC50	mortality	0.9	1, 2, 3	Lindgren *et al.*, 1954
Rhyzopertha dominica	2-6 wks			26	2 h	LC50	mortality	3.8	1, 2, 3	Lindgren *et al.*, 1954
Rhyzopertha dominica	2-6 wks			26	6 h	LC50	mortality	3.0	1, 2, 3	Lindgren *et al.*, 1954
Sitophilus granarius	adult			25	5 h	LC50	mortality	3.8	1	Bond & Monro, 1960
Sitophilus granarius	2-6 wks			26	2 h	LC50	mortality	14.0	1, 2, 3	Lindgren *et al.*, 1954
Sitophilus granarius	2-6 wks			26	6 h	LC50	mortality	3.0	1, 2, 3	Lindgren *et al.*, 1954
Sitophilus oryza	2-6 wks			26	2 h	LC50	mortality	14.0	1, 2, 3	Lindgren *et al.*, 1954
Sitophilus oryza	2-6 wks			26	6 h	LC50	mortality	2.6	1, 2, 3	Lindgren *et al.*, 1954
Stegobium paniceum	1-2 wks old			26	2 h	LC50	mortality	6.5	1, 2, 3	Lindgren *et al.*, 1954
Stegobium paniceum	1-2 wks old			26	6 h	LC50	mortality	2.8	1, 2, 3	Lindgren *et al.*, 1954
Tenebroides mauritanicus	4th instar larvae			25	5 h	LC50	mortality	13.5	1	Bond & Monro, 1960
Tribolium confusum	adult			25	5 h	LC50	mortality	3.5	1	Bond & Monro, 1960
Tribolium confusum	2-6 wks			26	2 h	LC50	mortality	12.5	1, 2, 3	Lindgren *et al.*, 1954
Tribolium confusum	2-6 wks			26	6 h	LC50	mortality	3.4	1, 2, 3	Lindgren *et al.*, 1954
Trogoderma granarium	diapause larvae			16-19.5	7 d	LC50	mortality	143.9	1, 4	Bains *et al.*, 1976
Zabrotes pectoralis	1-2 wks old			26	2 h	LC50	mortality	5	1, 2, 3	Lindgren *et al.*, 1954
Zabrotes pectoralis	1-2 wks old			26	6 h	LC50	mortality	2.2	1, 2, 3	Lindgren *et al.*, 1954

Notes
1 Closed system.
2 Experiment time 4 d.
3 During exposure T was 21ºC.
4 Exposure in airtight chamber.

Table A8. 3. Acute toxicity data methyl bromide to organisms exposed via air.

Species	Species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Insecta										
Acanthoscelides obtectus	1-2 weeks			26	2 h	LC50	mortality	9.0	1, 2, 12	Lindgren *et al*., 1954
Acanthoscelides obtectus	1-2 weeks			26	6 h	LC50	mortality	4.2	1, 2, 12	Lindgren *et al*., 1954
Callosobruchus chinensis	adult 1 d				24 h	LC50	mortality	1.67	1	Adu *et al.*, 1985
Callosobruchus chinensis	2-3 days old pupae				24 h	LC50	mortality	0.891	1	Adu *et al.*, 1985
Callosobruchus chinensis	larvae third instar				24 h	LC50	mortality	2.208	1	Adu *et al.*, 1985
Callosobruchus chinensis	eggs 1 d				24 h	LC50	mortality	0.851	1	Adu *et al.*, 1985
Corcyra cephalonica	eggs 1 d			26 ± 1	5 h	LC50	mortality	1.8	1, 10, 11	El-Buzz *et al*., 1974
Corcyra cephalonica	eggs 3 d			26 ± 1	5 h	LC50	mortality	1.7	1, 10, 11	El-Buzz *et al*., 1974
Corcyra cephalonica	larvae first instar			26 ± 1	5 h	LC50	mortality	1.1	1, 10, 11	El-Buzz *et al*., 1974
Corcyra cephalonica	larvae third instar			26 ± 1	5 h	LC50	mortality	1.4	1, 10, 11	El-Buzz *et al*., 1974
Corcyra cephalonica	larvae last instar			26 ± 1	5 h	LC50	mortality	1.7	1, 10, 11	El-Buzz *et al*., 1974
Corcyra cephalonica	pupae			26 ± 1	5 h	LC50	mortality	2.7	1, 10, 11	El-Buzz *et al*., 1974
Cydia pomonella L.	third instar			5.9	2 h	LC50	mortality	36.5	1, 13	Moffitt *et al.*, 1992
Cydia pomonella L.	third instar			11.9	2 h	LC50	mortality	37.2	1, 13	Moffitt *et al.*, 1992
Cydia pomonella L.	third instar			5.6	2 h	LC50	mortality	25.7	1, 14	Moffitt *et al.*, 1992
Cydia pomonella L.	third instar			11	2 h	LC50	mortality	26.9	1, 14	Moffitt *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	31.9	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	29.8	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	36.0	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	33.9	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	31.9	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	31.6	1, 15	Maindonald *et al.*, 1992
Cydia pomonella L.	eggs			12	2 h	LD50	mortality	29.4	1, 15	Maindonald *et al.*, 1992
Ephestia kuehniella	eggs 1d			26 ± 1	5 h	LC50	mortality	2.46	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 1d			26 ± 1	6 h	LC50	mortality	2.24	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 1d			26 ± 1	7 h	LC50	mortality	2.20	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 2 d			26 ± 1	5 h	LC50	mortality	2.28	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 2 d			26 ± 1	6 h	LC50	mortality	2.13	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 2 d			26 ± 1	7 h	LC50	mortality	2.08	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 3 d			26 ± 1	5 h	LC50	mortality	2.15	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 3 d			26 ± 1	6 h	LC50	mortality	2.05	1, 3	Mostafa *et al*., 1972
Ephestia kuehniella	eggs 3 d			26 ± 1	7 h	LC50	mortality	2.02	1, 3	Mostafa *et al*., 1972
Maconellicoccus hirsutus	eggs			25	2 h	LC50	mortality	7.1	1, 3, 9	Zettler *et al*., 2002
Maconellicoccus hirsutus	crawlers			25	2 h	LC50	mortality	25.1	1, 3, 9	Zettler *et al*., 2002
Maconellicoccus hirsutus	early nymphs			25	2 h	LC50	mortality	26.5	1, 3, 9	Zettler *et al*., 2002
Maconellicoccus hirsutus	late nymphs			25	2 h	LC50	mortality	25.0	1, 3, 9	Zettler *et al*., 2002
Maconellicoccus hirsutus	adult females			25	2 h	LC50	mortality	25.7	1, 3, 9	Zettler *et al*., 2002
Oryzaephilus surinamensis	2-6 weeks			26	2 h	LC50	mortality	17.0	1, 2, 12	Lindgren *et al*., 1954
Oryzaephilus surinamensis	2-6 weeks			26	6 h	LC50	mortality	4.4	1, 3, 12	Lindgren *et al*., 1954

Species	Species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Plodia interpunctella	larvae			26.5	4 h	LC50	mortality	5.5	1	Sardesai, 1972
Plodia interpunctella	diapausing larvae			26.5	4 h	LC50	mortality	10.4	1	Sardesai, 1972
Rhyzopertha dominica	2-6 weeks			26	2 h	LC50	mortality	11.0	1, 2, 12	Lindgren *et al*., 1954
Rhyzopertha dominica	2-6 weeks			26	6 h	LC50	mortality	3.4	1, 3, 12	Lindgren *et al*., 1954
Sitophilus granarius	2-6 weeks			26	2 h	LC50	mortality	18.5	1, 2, 12	Lindgren *et al*., 1954
Sitophilus granarius	2-6 weeks			26	6 h	LC50	mortality	4.8	1, 3, 12	Lindgren *et al*., 1954
Sitophilus granarius	adult			25	5 h	LC50	mortality	4.2	1, 3	Bond & Monro, 1960
Sitophilus oryza	2-6 weeks			26	2 h	LC50	mortality	9.5	1, 2, 12	Lindgren *et al*., 1954
Sitophilus oryza	2-6 weeks			26	6 h	LC50	mortality	3.6	1, 3, 12	Lindgren *et al*., 1954
Sitophilus oryza	eggs 1d			26 ± 1	5 h	LC50	mortality	6.19	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 1d			26 ± 1	6 h	LC50	mortality	5.97	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 1d			26 ± 1	7 h	LC50	mortality	5.71	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 2 d			26 ± 1	5 h	LC50	mortality	6.02	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 2 d			26 ± 1	6 h	LC50	mortality	5.88	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 2 d			26 ± 1	7 h	LC50	mortality	5.59	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 3 d			26 ± 1	5 h	LC50	mortality	5.85	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 3 d			26 ± 1	6 h	LC50	mortality	5.56	1, 3	Mostafa *et al*., 1972
Sitophilus oryza	eggs 3 d			26 ± 1	7 h	LC50	mortality	5.45	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 1d			26 ± 1	5 h	LC50	mortality	2.21	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 1d			26 ± 1	6 h	LC50	mortality	2.14	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 1d			26 ± 1	7 h	LC50	mortality	1.94	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 2 d			26 ± 1	5 h	LC50	mortality	2.13	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 2 d			26 ± 1	6 h	LC50	mortality	1.93	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 2 d			26 ± 1	7 h	LC50	mortality	1.91	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 3 d			26 ± 1	5 h	LC50	mortality	1.98	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 3 d			26 ± 1	6 h	LC50	mortality	1.87	1, 3	Mostafa *et al*., 1972
Sitotroga cerealella	eggs 3 d			26 ± 1	7 h	LC50	mortality	1.85	1, 3	Mostafa *et al*., 1972
Stegobium paniceum	1-2 weeks			26	2 h	LC50	mortality	15.5	1, 2, 12	Lindgren *et al*., 1954
Stegobium paniceum	1-2 weeks			26	6 h	LC50	mortality	4.4	1, 3, 12	Lindgren *et al*., 1954
Tenebroides mauritanicus	5 d eggs			25	5 h	LC50	mortality	4	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus	3rd instar larvae			25	5 h	LC50	mortality	12.5	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus	4th instar larvae			25	5 h	LC50	mortality	14.8	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus	pupa (3-5 days)			25	5 h	LC50	mortality	17.6	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus	adult (3-5 days)			25	5 h	LC50	mortality	16.7	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus	adult (2-4 weeks)			25	5 h	LC50	mortality	12.8	1, 3	Bond & Monro, 1960
Tenebroides mauritanicus (L.)	larvae	y		25	90 min	LD50	mortality	43.3	4, 4, 8	Monro *et al*., 1965
Tenebroides mauritanicus (L.)	larvae	y		25	90 min	LD50	mortality	25.5	4, 5, 8	Monro *et al*., 1965
Tribolium castaneum	eggs 1d			26 ± 1	5 h	LC50	mortality	3.92	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 1d			26 ± 1	6 h	LC50	mortality	3.61	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 1d			26 ± 1	7 h	LC50	mortality	3.42	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 2 d			26 ± 1	5 h	LC50	mortality	3.65	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 2 d			26 ± 1	6 h	LC50	mortality	3.44	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 2 d			26 ± 1	7 h	LC50	mortality	3.27	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 3 d			26 ± 1	5 h	LC50	mortality	3.38	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 3 d			26 ± 1	6 h	LC50	mortality	3.29	1, 3	Mostafa *et al*., 1972
Tribolium castaneum	eggs 3 d			26 ± 1	7 h	LC50	mortality	3.06	1, 3	Mostafa *et al*., 1972
Tribolium confusum	2-6 weeks			26	2 h	LC50	mortality	32.5	1, 2, 12	Lindgren *et al*., 1954
Tribolium confusum	2-6 weeks			26	6 h	LC50	mortality	9.2	1, 3, 12	Lindgren *et al*., 1954
Tribolium confusum	adults	y		25	90 min	LD50	mortality	23.7	4, 6, 8	Monro *et al*., 1965
Tribolium confusum	adults	y		25	90 min	LD50	mortality	21.5	4, 7, 8	Monro *et al*., 1965
Tribolium confusum	4-8 weeks			4	16 h	LD50	mortality	6.64	1, 3	Kenaga, 1960

Species	Species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Tribolium confusum	4-8 weeks			4	5 h	LD50	mortality	26.71	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			4	2 h	LD50	mortality	90.75	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			16	16 h	LD50	mortality	5.05	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			16	5 h	LD50	mortality	17.24	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			16	2 h	LD50	mortality	41.28	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			27	16 h	LD50	mortality	3.6	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			27	5 h	LD50	mortality	9.57	1, 3	Kenaga, 1960
Tribolium confusum	4-8 weeks			27	2 h	LD50	mortality	22.68	1, 3	Kenaga, 1960
Tribolium confusum	adult			25	5 h	LC50	mortality	9.0	1, 3	Bond & Monro, 1960
Zabrotes pectoralis	1-2 weeks			26	2 h	LC50	mortality	10.5	1, 2, 12	Lindgren *et al*., 1954
Zabrotes pectoralis	1-2 weeks			26	6 h	LC50	mortality	3.5	1, 3, 12	Lindgren *et al*., 1954

Notes
1 Closed system.
2 Experiment time 4 d.
3 In mg L^{-1}.
4 At 35mm Hg.
5 At 100 mm Hg.
6 At 75 mm Hg.
7 At 120 mm Hg.
8 Vacuum fumigation.
9 Concentration range: 8-64 mg L^{-1}.
10 Concentration range: 0.63-4.051 mg L^{-1}.
11 LC50 is range of 6 values; 6 different diets of parents, difference in diet results in a max. difference in LC50 value of a factor 1.3.
12 Exposure T was 21ºC.
13 Bing cherries.
14 Rainier cherries.
15 Different cherry cultivars.

Table A8. 4. Chronic toxicity data of 1,2-dibromoethane to organisms exposed via air.

Species	species properties	A	Substance purity	T [°C]	Exp. time	Criterion	Test endpoint	Value [mg.L^{-1}]	Notes	Reference
Fungi										
Verticillium dahliae	< 100 µM diameter			24	16 d	EC10	microsclerotia	424	1	Ben-Yephet *et al.*, 1981

Notes
1 Closed system.

Appendix 9 References to toxicity data

Anonymus. 2003. Regeling inzake milieukwaliteitseisen voor het Scheldebekken. Den Haag: Sdu Uitgevers. Staatscourant nr. 28. p. 23.

Anonymus. 2004. Substance Data Sheet: (5) Pentabromodiphenylether (penta-BDE). Schmallenberg, Germany: Fraunhofer Institute Molecular Biology and Applied Biology. Report no. Draft of 010304. 12 pp.

Anonymus. 2005. Environmental Quality Standards (EQS) Substance Data Sheet. Priority substance No. 25. Octylphenols (para-tert-octylphenol). Brussels, Belgium: Report no. Final. 18 pp.

Anonymus. Hazardous Substances Data Bank [Web Page] (Available at http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~Z57mxx:1) Accessed: 2005.

Anonymus. Syracuse Research Corporation. Physprop database [Web Page] (Available at http://www.syrres.com/esc/physdemo.htm) Accessed: June 10, 2005.

Anonymus. EDQM. European Pharmacopoeia Online, Ph. Eur. *5.2* [Web Page] (Available at http://online.pheur.org/NXT/gateway.dll?f=templates&fn=default.htm) Accessed: Sept. 8, 2005.

Anonymus. RIZA (Institute for Inland Water Management and Waste Water Treatment). Normen voor het waterbeheer. Tabellen [Web Page] (Available at http://www.rijkswaterstaat.nl/rws/riza/wateremissies/Thema/Normen_voor_het_waterbeheer/tabellen.html) Accessed: 2006.

Anonymus. RIZA (Institute for Inland Water Management and Waste Water Treatment). *Normen zoeksysteem* [Web Page] (Available at http://www.rijkswaterstaat.nl/rws/riza/wateremissies/Thema/Normen_voor_het_waterbeheer/normen.php) Accessed: 2006.

Anonymus. SPARC on-line calculator v3.1 [Web Page] (Available at http://ibmlc2.chem.uga.edu/sparc/index.cfm) Accessed: 2006 .

Anonymus. EPA. High Production Volume (HPV) Challenge Program. Robust summaries and test plans [Web Page] (Available at http://cfpub.epa.gov/hpv-s/) Accessed: Oct. 20, 2006.

Abdalla N, Lear B. 1975. Lethal dosages of methyl bromide for four plant-parasitic nematodes and the effect of soil temperature on its nematicidal activity. Plant Dis Rep 59: 224-228.

Adu OO, Muthu M. 1985. The relative toxicity of seven fumigants to life cycle stages of *Callosobruchus chinensis* (L). Insect Sci Appl 6: 75-78.

Alabaster JS. 1969. Survival of fish in 164 herbicides, insecticides, fungicides, wetting agents and miscellaneous substances. International Pest Control March/April: 29-35.

Aldenberg T, Jaworska JS. 2000. Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicol Environ Saf 46: 1-18.

Alexeeff GV, Kilgore WW, Li M. 1990. Ethylene dibromide: toxicology and risk assessment. Rev Environ Contam Toxicol 112: 49-122.

Andersen HR, Kjoholt J, Hansen M, Stuer-Lauridsen F, Dueholm Blicher T, Ingerslev F, Halling-Sorensen B. 2004 . Degradation of estrogens in sewage treatment processes. Denmark: Danish Environmental Protection Agency. Report no. 899. 61 pp.

Andersen HR, Wollenberger L, Halling-Sřrensen B, Kusk KO. 2001. Development of copepod nauplii to copepodites - a parameter for chronic toxicity including endocrine disruption. Environ Toxicol Chem 20: 2821-2829.

Anonymus. 1998. Besluit van 23 april 1998, houdende Warenwetbesluit Azo-kleurstoffen. 's-Gravenhage, the Netherlands: Sdu Uitgevers. Report no. 1998 339. 25 pp.

Anonymus. 2003. Besluit van 27 juni 2003 tot wijziging van het Warenwetbesluit Azo-kleurstoffen in verband met het beperken van de handel in en het gebruik van bepaalde gevaarlijke stoffen en

preparaten. 's-Gravenhage, the Netherlands: Sdu Uitgevers. Report no. 2003 296. 5 pp.
Appleton HT, Sikka HC. 1980. Accumulation, elimination and metabolism of dichlorobenzidine in the bluegill sunfish. Environ Sci Technol 14: 50-54.
ARCEM. 2003. Hormonwirksame Stoffe in Österreichs Gewässer - Ein Risiko? Wien, Austria: Umweltbundesamt GmbH. Report no. ISBN 3-85457-695-1. 462 pp.
Arildskov NP, Pedersen PG, Albrechtsen H-J. 2001. Fate of the herbicides 2,4,5-T, atrazine and DNOC in a shallow, anaerobic aquifer investigated by in sity passive diffusive emitters and laboratory batch experiments. Ground Water 39: 819-830.
ATSDR. 1992. Bromomethane. Agency for Toxic Substances and Disease Registry. Report no. TP-91/06. 104 pp.
ATSDR. 1998. 3,3'-Dichlorobenzidine (Update). Atlanta, Georgia, USA: Agency for Toxic Substances and Disease Registry. 145 pp.
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. Report no. 711701025. 297 pp.
Bains SS, Battu GS, Atwal AS. 1976. Efficacy of ethylene dibromide against diapause larvae of *Trogoderma granarium* everts at low temperature. Bull Grain Technol 14: 235-238.
Balch GC, Mackenzie CA, Metcalfe CD. 2004. Alterations to gonadal development and reproductive succes in Japanese medaka (*Oryzias latipes*) exposed to 17α-ethinylestradiol. Environ Toxicol Chem 23: 782-791.
Banerjee S, Sikka HC, Gray R, Kelly CM. 1978. Photodegradation of 3,3'-Dichlorobenzidine. Environ Sci Technol 12: 1425-1427.
Banerjee S, Yalkowsky SH, Valvani SC. 1980. Water solubillity and octanol/water partition coefficient of organics. Limitations of the solubility-partition coefficient correlation. Environ Sci Technol 14: 1227-1229.
Bearden AP, Schultz TW. 1998. Comparison of *Tetrahymena* and *Pimephales* toxicity based on mechanism of action. SAR QSAR Environ Res 9: 127-153.
Beek MA. 1999. Overzicht van ad hoc MTR's voor water. Lelystad: Institute for Inland Water Management and Waste Water Treatment. Report no. 99.046X. 23 pp.
Beek MA. 2002. Ad hoc MTR's voor de stoffen uit de Richtlijn 76/464/EEG. Lelystad: Institute for Inland Water Management and Waste Water Treatment. Report no. 2002.106X. 62 pp.
Behret H. 1987. Bromomethane. BUA Report 14 ed. Weinheim, Germany: VCH Verlagsgesellschaft mbH. 59 pp.
Behret H. 2001. BUA Report 223 (supplementary reports VII). Stuttgart, Germany: S. Hirzel Verlag.
Belfroid AC, Van der Horst A, Vethaak AD, Schäfer AJ, Rijs GBJ, Wegener J, Cofino WP. 1999. Analysis and occurence of estrogenic hormones and their glucuronides in surface water and waste water in The Netherlands. Sci Total Environ 225: 101-108.
Ben-Yephet Y, Letham D, Evans G. 1981. Toxicity of 1,2-dibromoethane and 1,3-dichloropropene to microsclerotia of *Verticillium dahliae*. Pestic Sci 12: 170-174.
Benson WH, Stackhouse RA. 1986. Evaluation of a new approach to the safety assessment of biomaterials. Drug Chem Toxicol 9: 275-183.
BioByte. 2004. BioLoom [computer program]. version 1.0 (ClogP 4.0). Claremont, CA, USA: BioByte Corporation.
Blum DJ, Speece RE. 1991. Quantitative structure-activity relationships for chemical toxicity to environmental bacteria. Ecotoxicol Environ Saf 22: 198-224.
Bláha L, Damborský J, Nemec M. 1998. PII: S0045-6535(97)10020-0 QSAR for acute toxicity of saturated and unsaturated halogenated aliphatic compounds. Chemosphere 36: 1345-1365.
Bond EJ, Monro HAU. 1961. The toxicity of various fumigants to the Cadelle, *Tenebroides*

mauritanicus. J Econ Entomol 54: 451-454.
Bontje D, Traas TP, Mennes W. 2005. A human exposure model to calculate harmonized risk limits. Bilthoven, the Netherlands: National Institute for Public Health and Environmental Protection. Report no. 601501022. 115 pp.
Boyd SA, Kao C-W, Suflita JM. 1984. Fate of 3,3'-dichlorobenzidine in soil: persistence and binding. Environ Toxicol Chem 3: 201-208.
Bridie AL, Wolff CJM, Winter M. 1979. The acute toxicity of some petrochemicals to goldfish. Water Res 13: 623-626.
Briggs GG. 1981. Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the Parachor. J Agric Food Chem 29: 1050-1059.
Bringmann G. 1973. Bestimmung der biologischen Schadwirkung wassergefährdender Stoffe aus der Hemmung der Glucose-Assimilation des Bakterium Pseudomonas . Zeitschrift für Wasser-Abwasser-Forschung 94: 366-369.
Bringmann G. 1975. Bestimmung der biologischen Schadwirkung wassergefährdender Stoffe aus der Hemmung der Zellvermehrung der Blaualge Microcystis. Gesundheits-Ingenieur 96: 238-241.
Bringmann G. 1978. Bestimmung der biologischen Schadwirkung wassergefährdender Stoffe gegen Protozoen I. Bakterienfressende Flagellaten (Modellorganismus: *Entosiphon sulcatum* Stein). Z Wasser-Abwasser-Forsch 11: 210-215.
Bringmann G, Kühn R. 1959. Vergleichende wasser-toxikologische Untersuchungen an Bakterien, Algen und Kleinkrebsen. Gesundheits-Ingenieur 80: 115-120.
Bringmann G, Kühn R. 1960. Vergleichende toxikologische Befunde an Wasser-Bakterien. Gesundheits-Ingenieur 81: 337-340.
Bringmann G, Kühn R. 1976. Vergleichende Befunde der Schadwirkung wassergefährdender Stoffe gegen Bakterien (*Pseudomonas putida*) und Blaualgen (*Microcystis aeruginosa*). GWF Wasser/Abwasser 117: 410-413.
Bringmann G, Kühn R. 1977. Befunde der Schadwirkung wassergefährdender Stoffe gegen *Daphnia magna*. Z Wasser-Abwasser-Forsch 10: 161-166.
Bringmann G, Kühn R. 1977. Grenzwerte der Schadwirkung wassergefährdender Stoffe gegen Bakterien (*Pseudomonas putida*) und Grünalgen (*Scenedesmus quadricauda*) im Zellvermehrungshemmtest. Z Wasser-Abwasser-Forsch 10: 87-98.
Bringmann G, Kühn R. 1978. Grenzwerte der Schadwirkung wassergefährdender Stoffe gegen Blaualgen (*Microcystis aeruginosa*) und Grünalgen (*Scenedesmus quadricauda*) im Zellvermehrungshemmtest. Vom Wasser 50: 45-60.
Bringmann G, Kühn R. 1979. Vergleich der toxischen Grenzkonzentrationen wassergefährdender Stoffe gegen Bakterien, Algen und Protozoen im Zellvermehrungshemmtest. Gesundheits-Ingenieur 100: 249-252.
Bringmann G, Kühn R. 1980. Bestimmung der biologischen Schadwirkung wassergefährdender Stoffe gegen Protozoen II. Bakterienfressende Ciliaten. Z Wasser-Abwasser-Forsch 13: 26-31.
Bringmann G, Kühn R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Res 14: 231-241.
Bringmann G, Kühn R. 1982. Ergebnisse der Schadwirkung wassergefährdender Stoffe gegen *Daphnia magna* in einem weiterentwickelten standardisierten Testverfahren. Z Wasser-Abwasser-Forsch 15: 1-6.
Bringmann G, Kühn R, Winter A. 1980. Bestimmung der biologischen Schadwirkung wassergefährdender Stoffe gegen Protozoen III. Saprozoische Flagellaten. Z Wasser-Abwasser-Forsch 13: 170-173.
Bringmann G, Kühn R. 1976. Vergleichende Befunde der Schadwirkung wassergefährdender Stoffe gegen Bakterien (*Pseudomonas putida)* und Blaualgen *(Microcystis aeruginosa)*. GWF-

Wasser/Abwasser 117: 410-413.
Bringmann G, Kühn R. 1978. Testing of substances for their toxicity threshold: model organisms *Microcystis* (*Diplocystis*) *aeruginosa* and *Scenedesmus quadricauda*. Mitt Internat Verein Limnol 21: 275-284.
Bringmann G, Kühn R. 1981. Vergleich der Wirkung von Schadstoffen auf flagellate sowie ciliate bzw. auf holozoische bakterienfressende sowie saprozoische Protozoen. GWF-Wasser/Abwasser 122: 308-313.
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.
Broholm MM, Tuxen N, Rügge K, Bjerg PL. 2001. Sorption and degradation of the herbicide 2-Methyl-4,6-dinitrophenol under aerobic conditions in a sandy aquifer in Vejen, Denmark. Environ Sci Technol 35: 4789-4797.
Brooke D, Johnson I, Mitchell R, Watts C. 2005. Environmental risk evaluation report: 4-tert-octylphenol. Bristol, UK: Environment Agency. Report no. ISBN 1 84432 410 9. 205 pp.
Brooke LT. 1991. Results of freshwater exposures with the chemicals atrazine, biphenyl, butachlor, cabaryl, carbazole, dibenzofuran, 3,3'-dichlorobenzidine, dichlorovos, 1,2-epoxyethylbenzene (styrene oxide), isophorone, isopropalin, oxychlordane, pentachloroanisole, propoxur (baygon), tetrabromobisphenol A, 1,2,4,5-tetrachlorobenzene, and 1,2,3-trichloropropane to selected freshwater organisms. Superior, WI, USA: University of Wisconsin-Superior, Lake Superior Research Institute. 109 pp.
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.
Cajina-Quezada M, Schultz TW. 1990. Structure-toxicity relationships for selected weak acid respiratory uncouplers. Aquat Toxicol 17: 239-252.
Call DJ, Poirier SH, Lindberg CA, Harting SL, Markee TP, Brooke LT, Zarvan N, Northcott CE. 1989. Toxicity of selected uncoupling and acetylcholinesterase-inhibiting pesticides to the fathead minnow (*Pimephales promelas*). In: Weigmann DL, ed. Pesticides in terrestrial and aquatic environments. Blacksburg, VA, USA: Virginia Polytechnic Institute and State University. p. 317-336.
Canton JH, Wegman RCC, Mathijssen-Spiekman EAM, Wammes JY. 1980. Hydrobiologisch-toxicologisch onderzoek met methylbromide. Bilthoven: RIVM. Report no. 105/80 CBS VI/RA.
Crommentuijn T, Kalf DF, Polder MD, Posthumus R, Van de Plassche EJ. 1997. Maximum permissible concentrations and negligible concentrations for pesticides. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601501 002. 174 pp.
Crommentuijn T, Kalf DF, Polder MD, Posthumus R, Van de Plassche EJ. 1997. Maximum permissible concentrations and negligible concentrations for pesticides. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601501 002 - Annexes.
CTB. 2005. Toelatingsbesluit betreffende Methylbromide 100 voor ruimteontsmetting. Wageningen, the Netherlands: Het College voor de toelating van bestrijdingsmiddelen. Report no. 6476 N.
CTB. Board for the authorisation of pesticides. *Pesticides database* [Web Page] (Available at http://www.ctb.agro.nl/) Accessed: Oct. 26, 2005.
Curtis C, Lima A, Lozano SJ, Veith GD. 1982. Evaluation of a bacterial bioluminescence bioassay as a method for predicting acute toxicity of organic chemicals to fish. Amererican Socierty for Testing and Materials. ASTM STP 766. 170-178 pp.

Davis JT, Hardcastle WS. 1959. Biological assay of herbicides for fish toxicity. Weed Sci 7: 397-404.

Dawson GW, Jennings A. 1975-1977. The acute toxicity of 47 industrial chemicals to fresh and saltwater fishes. J Hazard Mat 1: 303-318.

Dawson GW, Jennings AL, Drozdowski D, Rider E. 1975-1977. The acute toxicity of 47 industrial chemicals to fresh and saltwater fishes. J Hazard Mat 1: 303-318.

De Bruijn J, Busser F, Seinen W, Hermens J. 1989. Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the 'slow-stirring' method. Environ Toxicol Chem 8: 499-512.

De Winter-Sorkina R, Bakker MI, Wolterink G, Zeilmaker MJ. 2006. Brominated flame retardants: occurence, dietary intake and risk assessment. Bilthoven, The Netherlands: National Institute for Public Health and the Environment. Report no. 320100002. 85 pp.

Deneer JW, Sinnige TL, Seinen W, Hermens JLM. 1988. A quantitative structure-activity relationship for the acute toxicity of some epoxy compounds to the guppy. Aquat Toxicol 13: 195-204.

Devillers J, Meunier T, Chambon P. 1985. Intéret de la relation dose-effet-temps en écotoxicologie pour la détermination des différentes classes chmiques de toxiques. Techniques et sciences municipales - L'eau 80: 329-334.

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

Dobbs RA, Wang LW, Govind R. 1989. Sorption of toxic organic compounds on wastewater solids: correlation with fundamental properties. Environ Sci Technol 23: 1092-1097.

Donaldson FP, Nyman MC. 2005. Sorption of benzidine and 3,3'-dichlorobenzidine to lake sediments. 1. Conceptualization and development of a multiparameter model. Environ Toxicol Chem 24: 1022-1028.

Dutka BJ, Kwan KK. 1981. Comparison of three microbial toxicity screening tests with the microtox test. Bull Environ Contam Toxicol 27: 753-757.

EC. 1976. Council Directive of 4 May 1976 on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community (76/464/EEC). Brussels, Belgium: EC. L 129.

EC. 1988. Coucil Directive (88/347/EEC) of 16 June 1998 amending Annex II to Directive 86/280/EEC on limit values and qualtity objectives for discharges of certain dangerous substances included in List I of the Annex to Directive 76/464/EEC. Brussels, Belgium: EC. L 158. p. 35-41.

EC. 1999. 1999/164/EC: Commission Decision of 17 February 1999 concerning the non-inclusion of DNOC of active substance in Annex I to Council Directive 91/414/EEC and the withdrawal of authorisations for plant protection products containing this active substance (notified under document number C(1999) 332) (Text with EEA relevance). Brussels, Belgium: EC. L 054. p. 21-22.

EC. 2000. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. Brussels, Belgium: EC. L 327. p. 1-72.

EC. 2001. European Union Risk Assessment Report Diphenyl ether, pentabromo derivative, Volume 50. Hansen, B. G., Munn, S. J., Pakalin, S., Heidorn, C. J. A., Allanou, R., Scheer, S., Pellegrini, G., Vegro, S., Luotamo, M., De Bruijn, J., Berthault, F., Loonen, H., Vormann, K., Naughton, A., Anfossi, V., and Praderio, L. eds. Luxembourg: Office for Official Publications of the European Communities. Report no. EUR 19730. 282 pp.

EC. 2002. European Union Risk Assessment Report 4-Nonylphenol (branched) and nonylphenol, Volume 10. Hansen, B. G., Munn, S. J., De Bruijn, J., Pakalin, S., Luotamo, M., Berthault, F., Vegro, S., Heidorn, C. J. A., Pellegrini, G., Vormann, K., Allanou, R., and Scheer, S. eds.

Luxemburg: Office for Official Publications of the European Communities. Report no. EUR 20387 EN. 227 pp.
EC. 2004. European Union Risk Assessment Report aniline, Volume 50. Munn, S. J., Allanou, R., Aschberger, K., Berthault, F., De Bruijn, J., Musset, S., O'Connor, S., Pakalin, S., Pellegrini, G., Scheer, S., and Vegro, S. eds. Luxembourg: Office for Official Publications of the European Communities. Report no. EUR 21092. 222 pp.
EC. 2004. EUSES 2.0, the European Union System for the Evaluation of Substances [computer program]. version 2.0.3. Bilthoven, The Netherlands: Prepared by the National Institute for Public Health and the Environment (RIVM) for the European Chemicals Bureau.
EC. 2005. Proposal for a Directive of the European Parliament and of the Coucil on environmental quality standards and pollution control in the field of water policy and amending Directive 2000/6-/EC. Brussels, Belgium: EC. p. 1-25.
EC. 2006. European Union Risk Assessment Report Coal-tar pitch, high temperature. Luxemburg: Office for Official Publications of the European Communities. Report no. draft.
EC-JRC. 2003. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commision 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.
ECB. 2000. IUCLID Dataset - 1-chloro-2,3-epoxypropane. Ispra, Italy: EC. 94 pp.
ECB. 2000. IUCLID Dataset - 3,3'-dichlorobenzidine. Ispra, Italy: EC. 56 pp.
ECB. 2000. IUCLID Dataset - dicofol. Ispra, Italy: EC. 84 pp.
ECB. 2000. IUCLID Dataset - N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD). Ispra, Italy: EC. 40 pp.
ECB. European Chemicals Bureau. *ESIS - European chemical Substances Information System* [Web Page] (Available at http://ecb.jrc.it/) Accessed: Sept. 8, 2005.
EG&G Bionomics. 1978. Acute toxicity of Santoflex 13 (BN-78-1384316) to the freshwater alga *Selenastrum capricornutum*. St. Louis, MO, USA: Monsanto. Report no. BP-78-9-152 (Project nr. H74-500). 10 pp.
El Buzz HK, Kamcl AH, El-Nahal AKM, El-Borollosy FM. 1974. Effect of diet on the susceptibility of the different developmental stages of *Corcyra Cephalonica* Staint. to carbon bisulphide and methyl bromide. Agric Res Rev (Cairo) 36: 21-29.
Eldred et al. 1999. Prediction of fathead minnow acute toxicity of organic compounds from molecular structure. Chem. Res. Toxicol 12:
EPA. 2003. Summaries. 793-24-8. 1,4-Benzenediamine, N-(1,3-dimethylbutyl)-N'-phenyl-. US EPA, website High Production Volume Challange Program: EPA. 34 pp.
EPA. 2004. EPI Suite™ [computer program]. version 3.12. U.S. Environmental Protection Agency; Office of Pollution Prevention Toxics and Syracuse Research Company.
Erickson SJ, Freeman AE. 1978. Toxicity screening of fifteen chlorinated and brominated compounds using four species of marine phytoplankton. In: Jolley RL, Gorchev H, Hamilton DH, eds. Water chlorination: Environmental Impact and health effects. Michigan: Ann Arbor Science. p. 307-310.
Escher BI, Bramaz N, Eggen RILRM. 2005. In vitro assessment of modes of toxic action of pharmaceuticals in aquatic life. Environ Sci Technol 39: 3090-3100.
Escher BI, Bramaz N, Mauer M, Richter M, Sutter D , Von Känel C, Zschokke M. 2005. Screening test battery for pharmaceuticals in urine and wastewater. Environ Toxicol Chem 24: 750-758.
Fayolle F. 1979. Consequences de l'apport de contaminants sur les lombriciens III. Essais de laboratoire. Doc Pédozoool 1: 34-65.
Finizio A, Vighi M, Sandroni D. 1997. Determination of n-octanol/water partition coefficient of

pesticide. Critical review and comparison of methods. Chemosphere 34: 131-161.
Freitag D, Ballhorn L, Geyer H, Korte F. 1985. Environmental hazard profile of organic chemicals. Chemosphere 14: 1589-1616.
Gälli R, Munz CD, Scholtz R. 1994. Evaluation and application of aquatic toxicity tests: use of the Microtox test for the prediction of toxicity based upon concentrations of contaminants in soil. Hydrobiologia 273: 179-189.
Garten CT. 1990. Multispecies methods of testing for toxicity: use of the Rhizobium-legume symbiosis in nitrogen fixation and correlations between responses by algae and terrestial plants. In: Wang W, Gorsuch JW, Lower WR, eds. Plants for toxicity assessment. Philadelphia, PA, USA: American Society for Testing and Materials. p. 69-84.
Garten CT, Trabalka JR. 1983. Evaluation of models for predicting terrestrial food chain behaviour of xenobiotics. Environ Sci Technol 17: 590-595.
GDCh, German Chemical Society-BUA. 1989. 3,3'-Dichlorobenzidine. Weinheim, Germany: VCH Verlagsgesellscharft mbH. Report no. BUA 30. 70, 72 pp.
GDCh, German Chemical Society-BUA. 1992. Epichlorohydin (1-chloro-2,3,epoxypropane). Stuttgart Germany: S. Hirzel Wissenschaftliche Verlagsgesellschaft. Report no. BUA 90. 132 pp.
GDCh, German Chemical Society-BUA. 1998. N-Isopropyl-N'-phenyl-1,4-phenylene diamine (IPPD) and N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylene diamine (6PPD). Stuttgart, Germany: S. Hirzel. Report no. BUA 207 and BUA 208. 70, 72 pp.
GDCh, German Chemical Society-BUA. 1999. Tris(2-chloroethyl)phosphate (No. 20), 3,3'-Dichorobenzidine (No. 30), Hexachloroethane (No. 34), 2-Chloro-4-nitroaniline (No. 43), 1,2-Dibromoethane (No. 66), Methallyl chloride (No. 109), Ethyl acrylate (No. 128), Tetramethyllead/Tetraethyllead (No. 130), Acrolein (No. 157), Thiourea (No. 179). Weinheim, Germany: VCH Verlagsgesellscharft mbH. Report no. BUA 223 (Supplementary reports VII).
Geiger DL, Call DJ, Brooke LT, Eds. 1988. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*). Volume IV. Superior, WI, USA: Center for Lake Superior Environmental Studies. 355 pp.
Geiger DL, Northcott CE, Call DJ, Brooke LT, Eds. 1985. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*). Volume II. Superior, WI, USA: Center for Lake Superior Environmental Studies. 326 pp.
Gersich FM, F.A. Blanchard, S.L. Applegath, C.N. Park. 1986. The precision of Daphnid (Daphnia magna Straus, 1820) static acute toxicity tests. Arch Environ Contam Toxicol 15: 741-749.
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.
Ghillebaert F, Chaillou C, Deschamps F, Roubaud P. 1995. Toxic effects, at three pH levels, of two reference molecules on common carp embryo. Ecotoxicol Environ Saf 32: 19-28.
Goodwin KD, Varner RK, Crill PM, Oremland RS. 2001. Comsumption of troposheric levels of methyl bromide by C_1 compound-utilizing bacteria and comparison to saturation kinetics. Appl Environ Microbiol 67: 5437-5443.
Government of Canada. 1993. Canadian Environmental Protection Act. Priority substances list assessment report. 3,3-Dichlorobenzidine. Ottawa, Ontario, Canada: Minister of Supply and Services Canada. Report no. En40-215/15E. 17 pp.
Government of Canada. 1994. Canadian Environmental Protection Act. Priority substances list assessment report. Aniline. Ottawa, Ontario, Canada: Minister of Supply and Services. Report no. En40-215/35E. 30 pp.
Gälli R, Munz CD, Scholtz R. 1994. Evaluation and application of aquatic toxicity tests: use of the Microtox test for the prediction of toxicity based upon concentrations of contaminants in soil. Hydrobiologia 273: 179-189.

Gälli R, Munz CD, Scholtz R. 1994. Evaluation and application of aquatic toxicity tests: use of the Microtox test for the prediction of toxicity based upon concentrations of contaminants in soil. Hydrobiologia 273: 179-189.

Haderlein SB, Schwarzenbach RP. 1993. Adsorption of substituted nitrobenzenes and nitrophenols to mineral surfaces. Environ Sci Technol 27: 316-326.

Haderlein SB, Weissmahr KW, Schwarzenbach RP. 1996. Specific adsorption of nitroaromatic explosives and pesticides to clay minerals. Environ Sci Technol 30: 612-622.

Hansler R, Posthumus R. In prep. Indicatieve milieukwaliteitsnormen voor prioritaire stoffen. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503025.

Hansler R, Traas TP, Mennes WC. 2006. Handreiking voor de afleiding van indicatieve milieukwaliteitsnormen. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503024. 64 pp.

Harder, A. 2002. Assessment of the risk potential of reactive chemicals with multiple modes of toxic action. Thesis. Swiss Federal Institute of Technology (ETH) Zurich, pp.

Health Council of the Netherlands. 1999. Endocrine disruptors in ecosystems. Rijswijk, The Netherlands: Health Council. Report no. 1999/13.

Heimbach F. 1984. Correlations between three methods for determining the toxicity of chemicals to earthworms. Pestic Sci 15: 605-611.

Hendriks , Stouten. 1993. Monitoring ... Ecotoxicol Environ Saf

Hermens J, Canton H, Steyger N, Wegman R. 1984. Joint effects of a mixture of 14 chemicals on mortality and inhibition of reproduction of *Daphnia magna*. Aquat Toxicol 5: 315-322.

Herring CO, Adams JA, Wilson BA, Pollard Jr S. 1988. Dose-response studies using ethylene dibromide (EDB) in *Hydra oligactis*. Bull Environ Contam Toxicol 40: 35-40.

Hertel RF, Kielhorn T. 1995. Methyl bromide. Environmental Health Criteria 166. Hanover: World Health Organisation (WHO). 324 pp.

Hill Jr. RL, Janz DM. 2003. Developmental estrogenic exposure in zebrafish (*Danio rerio*): I. Effects on sex ratio and breeding succes. Aquat Toxicol 63: 417-429.

Holcombe GW, Benoit DA, Hammermeister DE, Leonard EN, Johnson RD. 1994. Acute and long-term effects of nine chemicals on the japanese medaka (*Oryzia latipes*). Arch Environ Contam Toxicol 28: 287-297.

Holthaus KIE, Johnson AC, Jürgens MD, Williams RJ, Smith JJL, Carter JE. 2002. The potential for estradiol and ethinylestradiol to sorb to suspended and bed sediments in some English rivers. Environ Toxicol Chem 21: 2526-2535.

Hutchinson TH, Pounds NA, Hampel M, Williams TD. 1999. Impact of natural and synthetic steroids on the survival, development and reproduction of marine copepods (*Tisbe battagliai*). Sci Total Environ 233: 167-179.

IARC. 1979. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Sex Hormones (II). Lyon, France : WHO. Report no. Volume 21. 583 pp.

IARC. 1983. IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. Polynuclear aromatic compounds, Part1, Chemical, Environmental and Experimental Data. World Health Organisation. Report no. Volume 32; ISBN 92 832 1532 X. 477 pp.

IARC. 1987. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42. Lyon, France : WHO. Report no. Volume 1 to 42, Supplement 7. 440 pp.

IARC. International Agency for Research on Cancer. *Summaries & evaluations: Oestrogens, steroidal (group 1). Evidence for carcinogenicity to humans (sufficient). Supplement 7* [Web Page] (Available at http://www.inchem.org/documents/iarc/suppl7/oestrogenssteroidal.html) Accessed: 1987.

IARC. 1999. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans.

Re-evaluation of Some Organic Chemicals, Hydrazine, and Hydrogen Peroxide. Lyon, France : WHO. Report no. Volume 71. 1589 pp.

IARC. 1999. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals. Lyon, France : WHO. Report no. Volume 15, Supplement 7.

INERIS. chimie.ineris.fr. *1,2-Dibromoethane* [Web Page] (Available at http://chimie.ineris.fr/en/lien/basededonnees/environnementale/recherche/dossiers.php?id=644) Accessed: 2005.

INERIS. *Epichlorohydrine (106-89-8)* [Web Page] (Available at www.chimie.ineris.fr) Accessed: Oct. 28, 2005.

INERIS. 2006. Détermination des CE50 pour trois substances chimiques sans PNEC (2-Amino-4-Chlorophenol ; 2-Chloro-p-Toluidine ; Epichlorohydrine). Rapport d'essai. 6 février 2006. INERIS-DRC-06-66026-ECOT-VVE/FGO-n° 06CR012.doc.

IPCS. 1984. Environmental Health Criteria - Epichlorohydrin. Geneva, Switzerland: World Health Organization. Report no. 33. 51 pp.

IPCS. 1996. Environmental Health Criteria - 1,2-Dibromoethane. Geneva, Switzerland: World Health Organization. Report no. 177. 148 pp.

Jafvert CT. 1990. Sorption of organic acid compounds to sediments: intial model development. Environ Toxicol Chem 9: 1259-1268.

Jaser W, Severin GF, Jütting U, Jüttner I, Schramm K-W, Kettrup A. 2003. Effects of 17α-ethinylestradiol on the reproduction of the cladoceran species *Ceriodaphnia reticulata* and *Sida crystallina*. Environ Internat 28: 633-638.

JECFA. 2000. Estradiol-17-B, progesterone and testosterone. Toxicological evaluation of certain veterinary drug residues in food. Geneva, Switserland: World Health Organization (WHO) - IPCS: INternation Programme on Chemical Safety. Report no. WHO food additives series 43.

Johnson WW, Finley MT. 1980. Handbook of acute toxicity of chemicals to fish and aquatic invertebrates. Washington, D.C., USA: United States Department of the Interior Fish and Wildlife Service. Report no. 137 (Resource Publication). 98 pp.

Juhnke I, Ludemann D. 1978. Ergebnisse der untersuchung von 200 chemischen verbindungen auf akute fischtoxizitat mit dem goldorfentest. Zeitschrift für Wasser-Abwasser-Forschung 5: 161-164.

Jürgens MD, Holthaus KIE, Johnson AC, Smith JJL, Hetheridge M, Williams RJ. 2002. The potential for estradiol and ethinylestradiol degradation in english rivers. Environ Toxicol Chem 21: 480-488.

Jürgens MD, Johnson AC, Williams RJ. 1999. Fate and behavior of steriod estrogens in rivers: A scoping study R&D technical report. UK: Environment Agency. Report no. P161.

Kaiser KLE, Ribo JM. 1988. *Photobacterium phosphoreum* toxicity bioassay. II. Toxicity data compilation . Toxic Assess Internat J 3: 195-237.

Kenaga EE. 1961. Time, temperature and dosage relationships of several insecticidal fumigants. J Econ Entomol 54: 537-542.

Kopf W. 1995. Wirkung endokriner Stoffe in Biotests mit Wasserorganismen. Vortrag bei der 50. Fachtagung des Bay. LA für Wasserwirtschaft: Stoffe mit endokriner Wirkung im Wasser (abstract) (in German) 82-100.

Krijgsheld KR, Van der Gen A. 1986. Assessment of the impact of the emission of certain organochlorine compounds on the aquatic environment. Part III: Epichlorohydrin. Chemosphere 15: 881-893.

Kristensen T, Baatrup E, Bayley M. 2005. 17α-ethinylestradiol reduces the competitive reproductive fitness of the male guppy (*Poecilia reticulata*). Biol Reprod 72: 150-156.

Kszos LA, Talmage SS, Morris GW, Konetsky BK, Rottero T. 2003. Derivation of aquatic

screening benchmarks for 1,2-dibromoethane. Arch Environ Contam Toxicol 45: 66-71.
Kühn R, Pattard M. 1990. Results of the harmfull 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 K-L, Winter A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to *Daphnia magna*. Water Res 23: 495-499.
Lahnsteiner F, Berger B, Grubinger F, Weismann T. 2005. The effect of 4-nonylphenol on semen quality, viability of gametes, fertilization succes, and embryo and larvae survival in rainbow *(Oncorhynchus mykiss*). Aquat Toxicol 297-306.
Lai KM, Johnson KL, Scrimshaw MD, Lester JN. 2000. Binding of waterborne steroid estrogens to solid phases in river and estuarine systems. Environ Sci Technol 34: 3890-3894.
Landau M, Tucker Jr JW. 1984. Acute toxicity of EDB and aldicarb to young of two estuarine fish species. Bull Environ Contam Toxicol 33: 127-132.
Lange M, Gebauer W, Markl J, Nagel R. 1995. Comparison of testing acute toxicity on embryo of zebrafish, *Brachydanio rerio* and RTG-2 cytotoxicity as possible alternatives to the acute fish test. Chemosphere 30: 2087-2102.
Layton AC, Gregory BW, Seward JR, Schultz TW, Sayler GS. 2000. Mineralization of steroidal hormones by biosolids in wastewater treatment systems in Tennessee U.S.A. Environ Sci Technol 34: 3925-3931.
Leblanc GA. 1980. Acute toxicity of priority pollutants to water flea (*Daphnia magna*). Bull Environ Contam Toxicol 24: 684-691.
Lee LS, Nyman AK, Nyman MC, Jafvert C. 1997. Initial sorption of aromatic amines to surface soils. Environ Toxicol Chem 16: 1575-1582.
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). Schmallenberg, Germany: Fraunhofer-Institute Molecular Biology and Applied Biology. 47 pp.
Lide DR, Ed. 1997. Handbook of Chemistry and Physics. 78 ed. Boca Raton, USA: CRC Press LLC.
Liebig M, Egeler P, Oehlmann J, Knacker T. 2005. Bioaccumulation of ^{14}C-17α-ethinylestradiol by the aquatic oligochaete *Lumbriculus variegatus* in spiked artifical sediment. Chemosphere 59: 271-280.
Life System I. 1992. Toxicological profile for bromoethane. USA: U.S. Department of Health & Human Services. Report no. TP-91/06. 104 pp.
Lindgren DL, Vincent LE, Krohne HE. 1954. Relative effectiveness of ten fumigants to adults of eight species of stored-product insects. J Econ Entomol 47: 923-926.
Lipnick RL, K.R. Watson, A.K. Strausz. 1987. A QSAR study of the acute toxicity of some industrial organic chemicals to goldfish. Narcosis, electrophile and proelectrophile mechanisms. Xenobiotica , 17: 1011-1025.
Lobo RA, Stanczyk FZ. 1994. New knowledge in the physiology of hormonal contraceptives . Am J Obstet Gynecol 170: 1499-1507.
Luttik R, Linders J. 1990. DNOC (definitieve versie; M-75). Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 88/678801/064. 36 pp.
Lysak A, Marcinek J. 1972. Multiple toxic effect of simultaneous action of some chemical substances on fish. Rocz. Nauk. Roln. 94: 53-63.
Länge R, Hutchinson TH, Croudace CP, Siegmund F, Schweinfurth H, Hampe P, Panter GH, Sumpter JP. 2001. Effects of the synthetic estrogen 17α-ethinylestradiol on the life-cycle of the fathead minnow (*Pimephales promelas*). Environ Toxicol Chem 20: 1216-1227.
Mackay D, Shiu W-Y, Ma K-C. Physical-chemical properties and environmental fate. Handbook. CD-ROM. 2000. Chapman & Hall/CRC*net*BASE.
Maindonald JH, Waddell BC, Birtles DB. 1992. Response to methyl bromide fumigation of codling

moth (Lepidoptera: Tortricidae) eggs on cherries. J Econ Entomol 85: 1222-1230.
Malkomes H-P. 1990. Einfluss unterschiedlich formulierter Pflanzenschutzmittel auf mikrobielle Aktivitäten im Boden. J Plant Dis Protect 97: 517-531.
Malkomes H-P. 1999. Die erhöhung mikrobieller Aktivitäten im Boden durch Luzernemehl als Indikator ökotoxischer Wirkungen von Pflanzenschutzmitteln. Teil II: Beispiele mit underschiedlich wirksamen Pflanzenschutzmitteln. Agribiological Research-Zeitschrift für Agrarbiologie Agrikulturchemie Ökologie 52: 323-336.
Malkomes H-P. 1999. Die erhöhung mikrobieller Aktivitäten im Boden durch Luzernemehl als Indikator ökotoxischer Wirkungen von Pflanzenschutzmitteln. Teil I: Eignung verschiedener mikrobieller Aktivitäten. Agribiological Research-Zeitschrift für Agrarbiologie Agrikulturchemie Ökologie 52: 311-321.
Mayer Jr. FL, Ellersieck MR. 1986. Manual of acute toxicity: Interpretation and data base for 410 chemicals and 66 species of freshwater animals. Resource Publication 160 ed. Washington, DC, USA: United States Department of the interior fish and wildlife service.
Mayes MA, Alexander HC, Dill DC. 1983. A study to assess the influence of age on the response of fathead minnows in static acute toxicity tests. Bull Environ Contam Toxicol 31: 139-147.
MDL INformation Systems I. 1997. ISIS™/Draw 2.1.3d.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1997. Voorkomen van kankerverwekkende azo-kleurstoffen in Nederland. Vooronderzoek naar de wenselijkheid van aanvullende regulering. Hoofdrapport. Amsterdam, the Netherlands: CREM. 54 pp.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1997. Voorkomen van kankerverwekkende azo-kleurstoffen in Nederland. Vooronderzoek naar de wenselijkheid van aanvullende regulering. Achtergrondrapport. Amsterdam, the Netherlands: CREM. 94 pp.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1998. Prevention of carcinogenic azo dyes in the Netherlands (Background report). Zoetermeer, The Netherlands: VROM. Report no. 1998/34B - Publicatiereeks Stoffen, Veiligheid, Straling. 90 pp.
Mensink JS, Looye KM, Van Westerhoven M, Fluitman A. 1998. Prevention of carcinogenic azo dyes in the Netherlands (Main report). Zoetermeer, The Netherlands: VROM. Report no. 1998/34A - Publicatiereeks Stoffen, Veiligheid, Straling. 50 pp.
Meregalli G, Ollevier F. 2001. Exposure of *Chironomus riparius* larvae to 17α-ethynylestradiol: effects on survival and mouthpart deformities. Sci Total Environ 269 : 157-161.
Metcalfe CD, Metcalfe TL, Kiparissis Y, Koenig BG, Khan C, Hughes RJ, Croley TR, March RE , Potter T. 2001. Estrogenic potency of chemicals detected in sewage treatment plant effluents as determined by in vivo assays with Japanese medaka (*Oryzias latipes*). Environ Toxicol Chem 20: 297-308.
Meylan W, Howard PH. 1992. Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ Sci Technol 26: 1560-1567.
Moffitt HR, Drake SR, Toba HH, Hartsell PL. 1992. Comparative efficacy of methyl bromide against codling moth (Lepidoptera: Tortricidae) larvae in 'Bing' and 'Rainier' cherries and confirmation of efficacy of a quarantine treatment for 'Rainier' cherries. J Econ Entomol 85: 1855-1858.
Monro HAU, Dumas T, Buckland CT. 1965. The influence of vapour pressure of different fumigants on the mortality of two stored product insects in vacuum fumigation. J Stored Prod Res 1: 207-222.
Mostafa SAS, Kamel AH, El-Nahal AKM, El-Borollosy FM. 1972. Toxicity of carbon bisulphide and methyl bromide to eggs of four stored product insects. J Stored Prod Res 8: 193-198.
Nash JP, Kime DE, Van der Ven LTM, Wester PW, Brion F, Maack G, Stahlschmidt-Allner P, Tyler CR. 2004. Long-term exposure to environmental concentrations of pharmaceutical ethynylestradiol causes reproductive failure in fish. Environ Health Perspec 112: 1725-1733.
Nendza M, Seydel JK. 1988. Quantitative structure-toxicity relationships and multivariate data

analysis for ecotoxic chemicals in different biotestsystems. Chemosphere 17: 1575-1584.
Newman MC, Ownby DR, Mézin LCA, Powell DC, Christensen TRL, Lerberg SB, Anderson B-A. 2000. Applying species-sensitivity distributions in ecological risk assessment: assumptions of distribution type and sufficient numbers of species. Environ Toxicol Chem 19: 508-515.
Nyman MC, Haber KS, Kentämaa HI, Blatchley III ER. 2002. Photodechlorination of 3,3'-dichlorobenzidine in water. Environ Toxicol Chem 21: 500-506.
Nyman MC, Harden J, Nies LF, Blatchley III ER. 2004. Biodegradation of 3,3'-dichlorobenzidine in freshwater lake sediments. J Environ Eng Sci 3: 89-95.
Nyman MC, Nyman AK, Lee LS, Nies LF, Blatchley III ER. 1997. 3,3'-Dichlorobenzidine transformation processes in natural sediments. Environ Sci Technol 31: 1068-1073.
O'Connor OA, Young LY. 1989. Toxicity and anaerobic biodegradability of substituted phenols under methanogenic conditions. Environ Toxicol Chem 8: 853-862.
OECD. 1984. Alga, growth inhibition test. Paris, France: OECD. Report no. 201. 14 pp.
OECD. 1995. SIDS Initial assessment report for SIAM 3. PHENOL, 4-(1,1,3,3-TETRAMETHYLBUTYL)-. Williamsburg, VI, USA: OECD. 54 pp.
OECD. 2002. SIDS Initial assessment report for 13th SIAM Methyl bromide. Paris, France: OECD. 31 pp.
OECD. 2004. SIDS Initial assessment report for SIAM 18. N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylendiamine (6PPD). Paris, France: OECD. 36 pp.
Okkerman PC, Van de Plassche EJ, Slooff W, Van Leeuwen CJ, Canton JH. 1991. Ecotoxicological effects assessment: a comparison of several extrapolation procedures. Ecotoxicol Environ Saf 21: 182-193.
Ononye AI, Graveel JG. 1994. Modeling the reactions of 1-naphthylamine and 4-methylaniline with humic acids: spectroscopic investigations of the covalent linkages. Environ Toxicol Chem 13: 537-541.
OSPAR Commission. 2005. OSPAR background document on 4-(dimethylbutylamino)diphenylamine (6PPD). OSPAR Commission. Report no. 2005/228; ISBN 1-904426-63-8. 26 pp.
Park BJ, Kidd K. 2005. Effects of the synthetic estrogen ethinylestradiol on early life stages of mink frogs and green frogs in the wild and in situ. Environ Toxicol Chem 24: 2027-2036.
Parrott JL, Blunt BR. 2005. Life-cycle exposure of fathead minnows (*Pimephales promelas*) to an ethinylestradiol concentration below 1 ng/L reduces egg fertilization success and demasculinizes males. Environ Toxicol 20: 131-141.
Pascoe D, Carroll K, Karntanut M, Watts M. 2002. Toxicity of 17α-ethinylestradiol and bisphenol A to the freshwater cnidarian *Hydra vulgaris* . Arch Environ Contam Toxicol 43: 56-63.
Pawlowski S, Van Aerle R, Tyler CR, Braunbeck T. 2004. Effects of 17α-ethinylestradiol in a fathead minnow (*Pimephales promelas*) gonadal recrudescence assay. Ecotoxicol Environ Saf 57: 330-345.
Phipps GL, Holcombe GW, Fiandt JT. 1981. Acute toxicity of phenol and substituted phenols to the fathead minnow. Bull Environ Contam Toxicol 26: 585-593.
Pounds NA, Hutchinson TH, Williams TD, Whiting P, Dinan L. 2002. Assessment of putative endocrine disrupters in an in vivo crustacean assay and an in vitro insect assay . Mar Environ Res 54: 709-713.
Radix P, Léonard M, Papantoniou C, Roman G, Saouter E, Gallotti-Schmitt S, Thiébaud H, Vasseur P. 1999. Comparison of Brachionus calcyflorus 2-d and Microtox® chronic 22-h tests with Daphnia magna 21-d test for the chronic toxicity assessment of chemicals. Environ Toxicol Chem 18: 2178-2185.
Radix P, Severin G., Schramm KW, Kettrup A. 2002. Reproduction disturbances of *Brachionus calcyflorus* (rotifer) for the screening of environmental endocrine disrupters. Chemosphere 47: 1097-1101.

RIVM. National Institute for Public Health and the Environment. *Risico's van stoffen* [Web Page] (Available at http://www.rivm.nl/rvs/XML_normen/NormSearchResult.jsp?stof=534-52-1&norm=milieukwaliteit) Accessed: Mar. 9, 2006.

Sabljić A, Güsten H, Verhaar H, Hermens J. 1995. QSAR modelling of soil sorption. Improvements and systematics of log K_{oc} vs. log K_{ow} correlations. Chemosphere 31: 4489-4514.

Saito H, Koyasu J, Yoshida K, Shigeoka T, Koike S . 1993. Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. Chemosphere 25: 1015-1028.

Sanders HO, Cope OB. 1968. The relative toxicities of several pesticides to naiads of three species of stoneflies. Limnol Oceanogr 13: 112-117.

Sardesai JB. 1972. Response of diapausing and nondiapausing larvae of *Plodia interpunctella* to hydrogen cyanide and methyl bromide. J Econ Entomol 65: 1562-1565.

Sarmah AK, Northcott GL. 2006. Effect of organic carbon removal on sorption of steroid hormones by three New Zealand soils. In: Anonymus SETAC Europe.

Scholz S, Gutzeit HO. 2000. 17-α-ethinylestradiol affects reproduction, sexual differentiation and aromatase gene expression of the medaka (*Oryzias latipes*). Aquat Toxicol 50: 363-373.

Schulte C, Nagel R. 1994. Testing acute toxicity in the embryo of zebrafish, Brachydanio rerio, as an alternative to the acute fish test: preliminary results. ATLA 22: 12-19.

Schulte-Oehlmann U, Oetken M, Bachmann J, Oehlmann J. 2004. Effects of ethinylestradiol and methyltestosterone in prosobranch snails. In: Kümmerer K, ed. Pharmaceuticals in the environment. Sources, fate, effects and risks. Berlin, Heidelberg: Springer-Verlag. p. 233-247.

Schultz IR, Skillman A, Nicolas J-M, Cyr DG, Nagler JJ. 2003. Short-term exposure to 17α-ethylynestradiol decreases the fertility of sexually maturing male rainbow trout (*Oncorhychus mykiss*). Environ Toxicol Chem 22: 1272-1280.

Schultz TW. 1983. Aquatic toxicology of nitrogen heterocyclic molecules: quantitative structure-activity relationships. In: Nriagu JO, ed. Aquatic toxicology. New York, USA: John Wiley & Sons. p. 401-424.

Schultz TW. 1997. Tetratox: T*etrahymena 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 T*etrahymena pyriformis*. Chem Res Toxicol 12: 1262-1267.

Schultz TW, Bearden AP, Jaworska JS. 1996. A novel QSAR approach for estimating toxicity of phenols. SAR QSAR Environ Res 5: 99-112.

Schultz TW, Holcombe GW, Phipps GL. 1986. Relationships of quantitative structure-activity to comperative toxicity of selected phenols in the *Pimephales promelas* and T*etrahymena pyriformis* test systems. Ecotoxicol Environ Saf 12: 146-153.

Schultz TW, Sinks GD, Cronin MTD. 1997. Identification mechanisms of toxic action of phenols to *Tetrahymena pyriformis* from molecular descriptors. In: Schüürmann G, ed. Quantitative structure-activity relationships in environmental science. VII. Pensacola, FL, USA: SETAC Press. p. 329-342.

Schweinfurt H, Länge R, Miklautz H, Schauer G. Umweltverhalten und aquatische Toxizität von ethinylestradiol. 39-54.

Schäfers C, Teigeler M, Wenzel A, Maack G, Fenske M, Segner H. 2006. Concentration- and time-dependent effects of the synthetic estrogen, 17α-ethynylestradiol, on reproductive capabilities of the zebrafish, *Danio rerio*. Journal of Toxicology and Environmental Health (under revision)

Segers JHL, Temmink JHM, van den Berg JHJ, Wegman RCC. 1984. Morphological changes in the gill of carp (*Cyprinus carpio* L.) exposed to acutely toxic concentrations of methyl bromide. Water Res 18: 1437-1441.

Segner H, Caroll K, Fenske M, Janssen CR, Maack G , Pascoe D, Schäfers C, Vandenbergh GF, Watts M, Wenzel A. 2003. Identification of endocrine-disrupting effects in aquatic vertebrates

and invertebrates: report from the European IDEA project. Ecotoxicol Environ Saf 54: 302-314.
Seki M, Yokota H, Matsubara H, Tsuruda Y, Maeda M, Tadokoro H, Kobayashi K. 2002. Effect of ethinylestradiol on the reproduction and induction of vitellogenin and testis-ova in medaka (*Oryzias latipes*). Environ Toxicol Chem 21: 1692-1698.
Sekizawa J. 1996. 1,2-dibromoethane. Environmental Health Criteria 177 ed. Vammala, Finland: WHO, IPCS. 148 pp.
Sheng G, Johnston CT, Teppen BJ, Boyd SA. 2001. Potential contributions of smectite clays and organic matter to pesticide retention in soils. J Agric Food Chem 49: 2899-2907.
Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments. Athens, GA, USA: US-EPA. Report no. EPA-600/3-78-068. 49 pp.
Slooff W, Canton JH. 1983. Comparison of the susceptibility of 11 freshwater species to 8 chemical compounds. II. (Semi)chronic toxicity tests. Aquat Toxicol 4: 271-282.
Sparenburg P, Linders J. 1991. Dicofol (definitieve versie; M-84). Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 88/678801/092. 28 pp.
Thompson CM, McAllister WA, Forbis AD, Kaiser FE. 1979. Dynamic toxicity of Santoflex 13 (AB-78-121) to fathead minnows (*Pimephales promelas*). Flow-through bioassay final report. St. Louis, MI, USA: Monsanto (Performed at ABC Laboratories, Inc.). Report no. #21850-A/AB-780121B (Monsanto). Study of 12 pages, raw data included in Appendix 92 pages. 104 pp.
Tomlin CDS. The e-Pesticide Manual (Twelfth Edition). CD-ROM. 2002. Version: 2.2. The British Crop Protection Council.
Umwelt Bundes Amt. 1987. Luftqualitätskriterien für ausgwählte Umweltkanzerogene. Berlin, Germany: Erich Schmidt Verlag. Report no. Berichte 2/87. 280 pp.
Van den Belt K, Verheyen R, Witters H. 2001. Reproductive effects of ethynylestradiol and 4t-octylphenol on the zebrafish (*Danio rerio*). Arch Environ Contam Toxicol 41: 458-467.
Van den Belt K, Verheyen R, Witters H. 2003. Effects of 17α-ethynylestradiol in a partial life-cycle test with zebrafish (*Danio rerio*): effects on growth, gonads and female reproductive succes. Sci Total Environ 309: 127-137.
Van Vlaardingen PLA, Traas TP, Wintersen AM, Aldenberg T. 2004. *E_TX* 2.0 A program to calculate hazardous concentrations and fraction affected, based on normally distributed toxicity data. Bilthoven: National Institute for Public Health and the Environment. Report no. 601501028. 68 pp.
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) – Revision 2007. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601782001. 146 pp.
Verschaeve L, van Gompel J, Thilemans L, Regniers L, Vanparys P, van der Lelie D. 1999. VITOTOX® bacterial genotoxicity and toxicity test for the rapid sceening of chemicals. Environmental and Molecular Mutagenesis 33: 240-248.
Versonnen BJ, Janssen C.R. 2004. Xenoestrogenic effects of ethinylestradiol in zebrafish (*Danio rerio*). Environ Toxicol 19: 198-206.
Vethaak AD, Rijs GBJ, Schrap SM, Ruiter H, Gerritsen A, Lahr J. 2002. Estrogens and xeno-estrogens in the aquatic environment of the Netherlands. Occurence, potency and biological effects. Lelystad, The Netherlands: Dutch National Institute of Inland Water Management and Waste Water Treatment (RIZA) and the Dutch National Institute for Coastal and Marine Management (RIKZ). Report no. RIZA/RIKZ 2002.001.
Visser JT, Linders J. 1992. Methyl bromide. Bilthoven: RIVM. Report no. 91/670104/011. 35 pp.
Visser JT, Linders J. 1992. Methyl bromide (definitieve versie). Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 91/670104/011. 35 pp.
Wagner C, Løkke H. 1991. Estimation of ecotoxicological protection levels from NOEC toxicity

data. Water Res 25: 1237-1242.
Watts MM, Pascoe D, Carrol K. 2001. Survival and precopulatory behaviour of *Gammarus pulex* (L.) exposed to two zenoestrogens. Water Res 35: 2347-2352.
Weber EJ, Colón D, Baughman GL. 2001. Sediment-associated reactions of aromatic amines. 1. Elucidation of sorption mechanisms. Environ Sci Technol 35: 2470-2475.
Weissmahr KW, Haderlein SB, Schwarzenbach RP, Hany R, Nüesch R. 1997. In situ spectroscopic investigations of adsorption mechanisms of nitroaromatic compounds at clay minerals. Environ Sci Technol 31: 240-247.
Wellens H. 1982. Vergleich der Empfindlichkeit von Brachydanio rerio und Leuciscus idus bei der Untersuchung der Fischtoxizität von chemischen Verbindungen und Abwässern. Zeitschrift für Wasser-Abwasser-Forschung 15: 49-52.
Wester PW, Canton JH, Dormans JAMA. 1988. Pathological effect in freshwater fis *Poecilia reticulata* (guppy) and *Oryzias latipes* (medaka) following methyl bromide and sodium bromide exposure. Aquat Toxicol 12: 323-344.
Wester PW, Van der Heijden CA, Van Esch GJ. 1985. Carcinogenicity study with epichlorohydrin (CEP) by gavage in rats. Toxicology 36: 325-339.
WHO. 1998. Guidelines for Drinking-Water Quality - Second Edition - Volume 2 - Health Criteria and Other Supporting Information - Addendum. Geneva: World Health Organisation. Report no. WHO/EOS/98.1. 283 pp.
WHO. 2004. Epichlorohydrin in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. Geneva: World Health Organisation. 7 pp.
Young WF, Whitehouse P, Johnson I, Sorokin N. 2002. Proposed predicted no effect concentrations (PNECs) for natural and synthetic steroid oostrogens in surface waters. Report no. P2-T04/1.
Zeilmaker MJ, Kroese ED, Van Haperen P, Van Veen MP, Bremmer HJ, Van Kranen HJ, Wouters MFA, Janus JA. 1999. Cancer risk assessment of azo dyes and aromatic amines from garment and footwear. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503014. 51 pp.
Zeilmaker MJ, Van Kranen HJ, Van Veen MP, Janus JA. 2000. Cancer risk assessment of azo dyes and aromatic amines from tattoo bands, folders of paper, toys, bed clothes, watch straps and ink. Bilthoven, the Netherlands: National Institute for Public Health and the Environment. Report no. 601503019. 45 pp.
Zettler JL, Follett PA, Gill RF. 2002. Susceptibility of *Maconellicoccus hirsutus* (Homoptera: Pseudococcidae) to methyl bromide. J Econ Entomol 95: 1169-1173.
Zhang WM, McGiffen JR ME, Becker JO, Ohr HD, Sims JJ, Kallenbach RL. 1997. Dose response of weeds to methyl iodide and methyl bromide. Weed Res (Oxf) 37: 181-189.
Zillioux EJ, Johnson IC, Kiparissis Y, Metcalfe CD, Wheat JV, Ward SG, Liu H. 2001. The sheepshead minnow as an in vivo model for endocrine disruption in marine teleosts: A partial life-cycle test with 17α-ethynylestradiol. Environ Toxicol Chem 20: 1968-1978.
Zitko V, McLeese DW, Carson WG, Welch HE. 1976. Toxicity of alkyldinitrophenols to some aquatic organisms. Bull Environ Contam Toxicol 16: 508-515.
Zwolsman JJG, Bernhardi L, IJpelaar GF, van den Berg G.A. 2004. Bescherming drinkwaterfunctie - Bescherming van oppervlaktewater voor de drinkwatervoorziening onder de Europese Kaderrichtlijn Water. Rijswijk: VEWIN. Report no. 2004/43/4243. 48 pp.

Appendix 10 References of rejected toxicity data

Note: not all literature referenced in this section is shown in the toxicity tables with rejected studies.

Yang RSH, Witt KL, Alden CJ, Cockerham LG. 1995. Toxicology of Methyl Bromide. Rev Environ Contam Toxicol 142: 65-85.

Abdalla N, Lear B. 1975. Lethal dosages of methyl bromide for four plant-parasitic nematodes and the effect of soil temperature on its nematicidal activity. Plant Dis Rep 59: 224-228.

Adams JA, Kennedy AA. 1992. Sublethal Effects of Ethylene Dibromide on Wound Healing and Morphogenesis in *Hydra oligactis*. Arch Environ Contam Toxicol 22: 272-277.

Adams PM, Hanlon RT, Forsythe JW. 1989. Toxic Exposure to Ethylene Dibromide and Mercuric Chloride: Effects on Laboratory-Reared Octopuses. Neurotoxicol Teratol 10: 519-523.

Allen Y, Scott AP, Matthiessen P, Haworth S, Thain JE, Feist S. 1999. Survey of estrogenic activity in United Kingdom estuarine and coastal waters and its effects on gonadal development of the flounder *Platichthys flesus*. Environ Toxicol Chem 18: 1791-1800.

Arulgnanendran VGJ, Nirmalakhandan N. 1998. Microbial Toxicity in Soil Medium. Ecotoxicol Environ Saf 39: 48-56.

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

Blázquez M, Zanuy S, Carillo M, Piferrer F. 1998. Structural and functional effects of early exposure to estradiol-17β and 17α-ethynylestradiol on the gonads of the gonochoristic teleost *Dicentrarchus labrax*. 18: 37-47.

Bogers R, De Vries-Buitenweg S, Van Gils M, Baltussen E, Hargreaves A, Van de Waart B, De Roode D, Legler J, Murk A. 2006. Development of chronic tests for endocrine active chemicals Part 2: an extended fish early-life stage test with an androgenic chemical in the fathead minnow (*Pimephales promelas*). Aquat Toxicol 80: 119-130.

Bond EJ. 1951. The effect of methyl bromide on the respiration of the cadelle Tenebroides mauritanicus. Can J Zool 34: 405-415.

Bowry SK. 1985. A note on the effective dosages of some fumigants against certain stages of corcyra cephalonica staint II. East Afr Agric For J 51: 116-118.

Bowry SK. 1985. Relative toxicity of different fumigants against the adults of lesser grain border rizopertha dominica fabr and rice moth corcyra cephalonica staint. I. East Afr Agric For J 51: 101-107.

Brasfield SM, Weber LP, Talent LG, Janz DM. 2002. Dose-response and time course relationships for vitellogenin induction in male western fence lizards (*Sceloporus occidentalis*) exposed to ethinylestradiol. Environ Toxicol Chem 21: 1410-1416.

Brian JV, Augley JJ, Braithwaite VA. 2006. Endocrine disrupting effects on the nesting behaviour of male three-spined stickleback *Gasterosteus aculeatus* L. J Fish Biol 68: 1883-1890.

Bringmann G, Kühn R. 1977. Befunde der Schadwirkung wassergefährdender Stoffe gegen *Daphnia magna*. Z Wasser-Abwasser-Forsch 10: 161-166.

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

Canna-Michaelidou S. 1993. Microtox™ response to volatile organic pollutants - implementation of the test in investigating accidental or deliberate watersupply pollution. Sci Total Environ Supplement: 969-977.

Canton JH, Wegman RCC, Mathijssen-Spiekman EAM, Wammes JY. 1980. Hydrobiologisch-toxicologisch onderzoek met methylbromide. Bilthoven: RIVM. Report no. 105/80 CBS VI/RA.

Castro CE, Belser NO. 1978. Intoxication of *Aphelenchus Avenae* by Ethylene Dibromide.

Nematologica 24: 37-44.
Chung K-T, Chen S-C, Wong TY, Wei C-I. 1998. Effects of benzidine and benzidine analogues on growth of bacteria including *azotobacter vinelandII*. Environ Toxicol Chem 17: 271-275.
Critchley BR. 1972. Effects of Three Soil Fumigants on Carabidae. Plant Pathol (Oxf) 21: 188-194.
Cronin MTD, Dearden JC, Dobbs AJ. 1991. QSAR studies of comparative toxicity in aquatic organisms. Sci Total Environ 109: 431-439.
Darnerud PO, Lund B.-O., Brittebo EB, Brandt I. 1989. 1,2-Dirbromoethane and Chloroform in the rainbow trout (*Salmo Gairdneri*): Studies on distribution of nonvolatile and irreversibly bound metabolites. J Toxicol Environ Health 26: 209-221.
Dawson GW, Jennings AL, Drozdowski D, Rider E. 1975-1977. The acute toxicity of 47 industrial chemicals to fresh and saltwater fishes. J Hazard Mat 1: 303-318.
Devillers J, Flatin J. 2000. A general QSAR model for predicting the acute toxicity of pesticides to *Oncorhynchus Mykiss*. SAR QSAR Environ Res 11: 25-43.
Devillers J, Meunier T, Chambon P. 1985. Intéret de la relation dose-effet-temps en écotoxicologie pour la détermination des différentes classes chmiques de toxiques. Techniques et sciences municipales - L'eau 80: 329-334.
Dura G, Krasovski GN, Zholdakova ZI, Mayer G. 1985. Prediction of Toxicity Using Quantitative Structure-Activity Relationships. Arch Toxicol 8: 481-487.
ECB. 2000. IUCLID Dataset - N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD). Ispra, Italy: EC. 40 pp.
Erickson SJ, Hawkins CE. 1980. Effects of Halogenated Organic Compounds on Photosynthesis in Estuarine Phytoplankton. Bull Environ Contam Toxicol 24: 910-915.
Fenske M, Van Aerle R, Brack S, Tyler CR, Segner H. 2001. Development and validation of a homologous zebrafish (*Danio rerio* Hamilton-Buchanan) vitellogenin enzyme-linked immunosorbent assay (ELISA) and its application for studies on estrogenic chemicals. Comp Biochem Physiol, C: Comp Pharmacol Toxicol 129: 217-232.
Folmar LC, Hemmer M, Hemmer R, Bowman C, Kroll K, Denslow ND. 2000. Comparative estrogenicity of estradiol, ethynyl estradiol and diethylstilbestrol in an in vivo, male sheepshead minnow (*Cyprinodon variegatus*), vitellogenin bioassay. Aquat Toxicol 49: 77-88.
Folmar LC, Hemmer MJ, Denslow ND, Kroll K, Chen J, Cheek A, Richman H, Meredith H, Grau EG. 2002. A comparison of the estrogenic potencies of estradiol, ethynylestradiol, diethylstilbestrol, nonylphenol and methoxychlor in vivo and in vitro. Aquat Toxicol 60: 101-110.
Fournier J-C, Hormatallah A, Collu T, Froncek B. 1992. Labelling of microbial biomass with radioactive substrates as a means to estimate pesticide effects in soil. Sci Total Environ 123: 325-332.
Freitas dos Santos LM, Livingston AG. 1997. Mineralisation of 1,2-dibromoethane and other brominated aliphatics under aerobic conditions. Water Sci Technol 36: 17-25.
Freyberger A, Andrews P, Hartmann E, Eiben R, Loof I, Schmidt U, Temerowski M, Folkerts A, Becka M, Stahl B, Kayser M. 2003. Testing of endocrine active substances using an enhanced OECD test guideline 407: Experiences from studies on flutamide and ethinylestradiol. Pure Appl Chem 75: 2483-2489.
Froehner K, Meyer W, Grimme LH. 2002. Time-dependent toxicity in the long-term inhibition assay with *Vibrio fischeri*. Chemosphere 46: 987-997.
Gan J, Yates SR, Anderson MA, Spencer WF, Ernst FF, Yates MV. 1994. Effect of soil properties on degradation and sorption of methyl bromide in soil. Chemosphere 29: 2685-2700.
Garten CT. 1990. Multispecies methods of testing for toxicity: use of the Rhizobium-legume symbiosis in nitrogen fixation and correlations between responses by algae and terrestial plants. In: Wang W, Gorsuch JW, Lower WR, eds. Plants for toxicity assessment. Philadelphia, PA, USA: American Society for Testing and Materials. p. 69-84.

Gersich FM, F.A. Blanchard, S.L. Applegath, C.N. Park. 1986. The precision of Daphnid (Daphnia magna Straus, 1820) static acute toxicity tests. Arch Environ Contam Toxicol 15: 741-749.

Ghillebaert F, Chaillou C, Deschamps F, Roubaud P. 1995. Toxic effects, at three pH levels, of two reference molecules on common carp embryo. Ecotoxicol Environ Saf 32: 19-28.

Gibson R, Smith MD, Spary CJ, Tyler CR, Hill EM. 2005. Mixtures of estrogenic contaminants in bile of fish exposed to wastewater treatment works effluents. Environ Sci Technol 39: 2461-2471.

Grist EPM, Wells NC, Whitehouse P, Brighty G, Crane M. 2003. Estimating the effects of 17α-ethinylestradiol on populations of the fathead minnow *Pimephales promelas*:Are conventional toxicological endpoints adequate? Environ Sci Technol 37: 1609-1616.

Gutjahr-Gobell RE, Zaroogian GE, Borsay Horowitz DJ, Gleason TR, Mills LJ. 2006. Individual effects of estrogens on a marine fish, Cunner (*Tautogolabrus adspersus*), extrapolated to the population level. Ecotoxicol Environ Saf 63: 244-252.

Halfon E, Bruggemann R. 1989. Environmental hazard of eight chemicals present in the Rhine river. Water Sci Technol 21: 815-820.

Hall E, Sun B, Prakash J, Nirmalakhandan N. 1996. Toxicity of Organic Chemicals and Their Mixtures to Activated Sludge Microorganisms. J Environ Eng 122: 424-429.

Hall LW, Pinkney AE, Horseman LO. 1985. Mortality of Striped Bass Larvae in Relation to Contaminants and Water Quality in a Chesapeake Bay Tributary. Trans Am Fish Soc 114: 861-868.

Halling-Sorensen B, Nors Nielsen S, Lanzky PF, Ingerslev F, Holten Lützhoft HC, Jorgensen SE. 1998. Occurence, fate and effects of pharmaceutical substances in the environment - A review. Chemosphere 36: 357-393.

Harder A. 2002. Assessment of the risk potential of reactive chemicals with multiple modes of toxic action. Thesis. Swiss Federal Institute of Technology (ETH) Zurich, pp.

Hawkins WE, Walker WW, James MO, Manning CS, Barnes DH, Heard CS, Overstreet RM. 1998. Carcinogenic effects of 1,2-dibromoethane (ethylene dibromide; EDB) in Japanese medaka (*Oryzias latipes*). Mutat Res 399: 221-232.

Heberer T. 2002. Occurence, fate, and removal of pharmaceutical residues in the aquatic environment: a review of recent research data. Toxicol Lett 131: 5-17.

Hendricks JD, Shelton DW, Loveland PM, Pereira CB, Bailey GS. 1995. Carcinogenicity of Dietary Dimethylnitrosomorpholine, *N*-methyl-*N*'-Nitro-*N*-Nitrosoguanidine, and Dibromoethane in Rainbow Trout*1. Toxicol Pathol 23: 447-457.

Hense BA, Severin GF, Pfister G, Welzl G, Jaser W, Schramm KW. 2005. Effects of anthropogenic estrogens nonylphenol and 17α-ethinylestradiol in aquatic model ecosystems. Acta Hydroch Hydrobiol 33: 27-37.

Herring CO, Adams JA, Wilson BA, Pollard Jr S. 1988. Dose-response studies using ethylene dibromide (EDB) in *Hydra oligactis*. Bull Environ Contam Toxicol 40: 35-40.

Hole BD. 1981. Variation in tolerance of seven species of stored product Coleoptera to methyl bromide and phosphine in strains from twenty nine countries. Bull ent Res 71: 299-306.

Humphreys SDM, Rees HG, Routledge PA. 1999. 1,2-Dibromoethane - a toxicological review. Adverse Drug React Toxicol Rev 18: 125-148.

Jobling S, Sheahan D, Osborne JA, Matthiessen P, Sumpert JP. 1996. Inhibition of testicular growth in rainbow trout (*Oncorhychus mykiss*) exposed to estrogenic alkylphenolic chemicals. Environ Toxicol Chem 15: 194-202.

Juhnke I, Ludemann D. 1978. Ergebnisse der untersuchung von 200 chemischen verbindungen auf akute fischtoxizitat mit dem goldorfentest. Zeitschrift für Wasser-Abwasser-Forschung 5: 161-164.

Kaiser KLE, McKinnon MB, Fort FL. 1994. Interspecies toxicity correlations of rat, mouse and *Photobacterium Phosphoreum*. Environ Toxicol Chem 13: 1599-1606.

Kale P, Baum JW. 1979. Sensitivity of Drosophila melanogaster to Low Concentrations of the Gaseous 1,2-Dibromoethane: I. Acute Exposures. Environ Mutagen 1: 15-18.
Kelley WD, Rodriguez-Kabana R. 1979. Effects of sodium azide and methyl bromide on soil bacterial populations, enzymatic activities and other biological variables. Pestic Sci 10: 207-215.
Kime DE, Nash JP. 1999. Gamete viability as an indicator of reproductive endocrine disruption in fish. Sci Total Environ 233: 123-129.
Klöpffer W. 1992. Photochemical degradation of pesticides and other chemicals in the environment: a critical assessment of the state of the art. Sci Total Environ 123: 145-159.
Koch R. 1983. Molecular Connectivity Index for Assessing Ecotoxicological Behaviour of Organic Compounds. Toxicol Environ Chem 6: 87-96.
Koike H. 1961. The effects of Fumigants on Nitrate Production in Soil. Soil Sci Soc Am J 25: 204-206.
Korotkova GP, Tokin BP. 1968. Stimulation of the progess of somatic embryogenesis in some porifera and coelenterata. Acta Biol Acad Sci H 19: 465-474.
Kristen U, Kappler R. The Pollen Tube Growth Test. Methods Mol Biol 43: 189-198.
Labadie P, Budzinski H. 2006. Alteration of steroid hormone profile in juvenile tarbot (*Psetta maxima*) as a consequence of short-term exposure to 17alpha-ethynylestradiol. Chemosphere 64:
Lai KM, Scrimshaw MD, Lester JN. 2002. Biotransformation and bioconcentration of steroid estrogens by *Chlorella vulgaris*. Appl Environ Microbiol 68: 859-864.
Lai KM, Scrimshaw MD, Lester JN. 2002. Prediction of the bioaccumulation factors and body burden of natural and synthetic estrogens in aquatic organisms in the river systems. Sci Total Environ 289: 159-168.
Lange M, Gebauer W, Markl J, Nagel R. 1995. Comparison of Testing Acute Toxicity on Embryo of Zebrafish, *Brachydanio rerio* and RTG-2 Cytotoxicity as Possible Alternatives to the Acute Fish Test. Chemosphere 30: 2087-2102.
Larsson DGJ, Adolfsson-Erici M, Parkkonen J, Petterson M, Berg AH, Olsson P-E, Förlin L. 1999. Ethinyloestradiol - an undesired fish contraceptive? Aquat Toxicol 45: 91-97.
Leesch JG, Gillenwater HB, Woodward JO. 1974. Methyl bromide fumigation of shelled peanuts in bulk containers. J Econ Entomol 67: 769-771.
Liebig M, Egeler P, Oehlmann J, Knacker T. 2005. Bioaccumulation of ^{14}C-17α-ethinylestradiol by the aquatic oligochaete *Lumbriculus variegatus* in spiked artifical sediment. Chemosphere 59: 271-280.
Long PL, Burns Brown W, Goodship G. 1972. The effect of methyl bromide on coccidial oocysts determined under controlled conditions. Vet Rec 90: 562-565.
Ma T, Wan X, Huang Q, Wang Z, Liu J. 2005. Biomarker responses and reproductive toxicity of the effluent from a Chinese large sewage treatment plant in Japanese medaka (*Oryzias latipes*). Chemosphere 59: 281-288.
Majumder SK, Muthu M, Srinivasan KS, Natarajan CP, Bhatia DS, Subrahmanyan V. 1961. Studies on the storage of coffee beans-IV. Control of *Araecerus Fasciculatus* (DEG) in monsooned coffee and related storage experiments. Food Sci 332--339.
Malkomes H-P. 1995. Chemische Bodenentseuchung unter ökotoxikologischen Gesichtspunkten. I. Wirkung von Methylbromid auf mikrobielle Aktivitäten im Boden unter Freilandbedingungen. J Plant Dis Protect 102: 606-617.
Malkomes H-P. 1995. Chemische Bodenentseuchung unter ökotoxikologischen Gesichtspunkten. II. Folgewirkungen einer Freilandanwendung von Methylbromid auf mikrobielle Aktivitäten und deren Reaktion gegenüber Herbiziden. J Plant Dis Protect 103: 50-63.
Malkomes H-P. 2000. Vergleich des Einfusses unterschiedlich formulierter Herbizide auf mikrobielle Aktivitäten im Boden - eine Bestandsaufnahme. Z Pflanzenkr Pflanzenschutz 17:

781-789.
Martin JP. 1972. Side effects of organic chemicals on soil properties and plant growth. 733-792.
Mayes MA, Alexander HC, Dill DC. 1983. A study to assess the influence of age on the response of fathead minnows in static acute toxicity tests. Bull Environ Contam Toxicol 31: 139-147.
McCarthy LS, Mackay D, Smith AD, Ozburn GW, Dixon DG. 1993. Residue-Based Interpretation of Toxicity and Bioconcentration QSARs from Aquatic Bioassays: Polar Narcotic Organics. Ecotoxicol Environ Saf 25: 253-270.
Metcalfe CD, Metcalfe TL, Kiparissis Y, Koenig BG, Khan C, Hughes RJ, Croley TR, March RE , Potter T. 2001. Estrogenic potency of chemicals detected in sewage treatment plant effluents as determined by in vivo assays with Japanese medaka (*Oryzias latipes*). Environ Toxicol Chem 20: 297-308.
Milner CR, Goulder R. 1986. Comparitive Toxicity of Chlorophenols, Nitrophenols, and Phenoxyalkanoic Acids to Freshwater Bacteria. Bull Environ Contam Toxicol 37: 714-718.
Minton NA, Gillenwater HB. 1973. Methyl bromide fumigation of Pratylenchus brachyurus in Peanut shells. J Nematol 5: 147-149.
Mogensen BB, Spliid NH. 1995. Pesticides in Danish watercourses: occurrence and effects. Chemosphere 31: 3977-3990.
Mounat A, Hitier H. 1959. Essais de dinfection chimique des sols pour semis de tabac. Ann Exp Tabac Bergerac 3: 287-298.
Nimrod AC, Benson WH. 1998. Reproduction and development of Japanese medaka following an early life stage exposure to xenoestrogens. Aquat Toxicol 44: 141-156.
Nirmalakhandan N, Arulgnanendran V, Mohsin M, Sun B, Cadena F. 1994. Toxicity of mixtures of organic chemicals to microorganisms. Water Res 28: 543-551.
Nirmalakhandan N, Sun B, Arulgnanendran VJ, Mohsin M, Wang XH, Prakash J, Hall N. 1994. Analyzing and modeling toxicity of mixtures of organic chemicals to microorganisms. Water Sci Technol 30: 87-96.
Nyman MC, McCord K, Wood WL, Blatchley III ER. 2003. Transport behavior of 3,3'-dichlorobenzidine in a freshwater estuary. Environ Toxicol Chem 22: 20-25.
Ohr HD, Sims JJ, Grech NM, Becker JO, McGriffen MEJr. 1996. Methyl Iodide, an Ozone-Safe Alternative to Methyl Bromide as a soil Fumigant. Plant Dis 80: 731-735.
Olivier OJ, Jacobs G, Strydom DK. 1990. Effect of a foliar application of paclobutrazol in autmn on the reproductive development of 'Songold' plum. S-Afr Tydskr Plant Grond 7: 92-95.
Papoulias DM, Noltie DB, Tillitt DE. 1999. An in vivo model fish system to test chemical effects on sexual differentiation and development: exposure to ethinyl estradiol. Aquat Toxicol 48: 37-50.
Park D-S, Peterson C, Zhao S, Coats JR. 2004. Fumigation toxicity of volatile natural and synthetic cyanohydrins to stored-product pests and activity as soil fumigants. Pest Manag Sci 60: 833-838.
Peace J, Daniel D, Nirmalakhandan N, Egemen E. 1997. Predicting Microbial Toxicity of Nonuniform Multicomponent Mixtures of Organic Chemicals. J Environ Eng 123: 329-334.
Pignatello JJ. 1986. Ethylene Dibromide Mineralization in Soils under Aerobic Conditions. Appl Environ Microbiol 51: 588-592.
Pirselova K, Balaz S, Schultz TW. 1996. Model-Based QSAR for Ionizable Compounds: Toxicity of Phenols Against *Tetrahymena pyriformis*. Arch Environ Contam Toxicol 30: 170-177.
Poelarends GJ, Hylckama Vlieg JETv, Marchesi JR, Freitos dos Santos LM, Janssen DB. 1999. Degradation of 1,2-Dibromoethane by Mycobacterium sp. Strain GP1. J Bacteriol 181: 2050-2058.
Pradhan S, Bhambhani HJ, Wadhi SR. 1939. Fumigation of infested potatoes. Indian J Entomol 22: 181-189.
Prakash J, Nirmalakhandan N, Sun B, Peace J. 1996. Toxicity of binary mixtures of organic

chemicals to microorganisms. Water Res 30: 1459-1463.
Rodriguez-Kabana R, Kelley WD. Comparison of the nematicidal effects of sodium azide and methyl bromide in pine nursery beds. 2: 140.
Rodríguez-Kábana R, Robertson DG, King PS. 1987. Comparison of Methyl Bromide and Other Nematicides for Control of Nematodes in Peanut. Ann Appl Nematol 1: 56-58.
Rose J, Holbech H, Lindholst C, Norum U, Povlsden A , Korsgaard B, Bjerregaard P. 2002. Vitellogenin induction by 17β-estradiol and 17α-ethinylestradiol in male zebrafish (*Danio rerio*). Comp Biochem Physiol, C: Comp Pharmacol Toxicol 131: 531-539.
Rouard N, Dictor M-C, Chaussod R, Soulas G. 1996. Side-effects of herbicides on the size and activity of the soil microflora: DNOC as a test case. Eur J Soil Sci 47: 557-566.
Rousseaux S, Hartmann A, Rouard N, Soulas G. 2003. A simplified procedure for terminal restriction fragment length polymorphism analysis of the soil bacterial community to study the effects of pesticides on the soil microflora using 4,6-dinitroorthocresol as a test case. Biol Fertil Soils 37: 250-254.
Routledge EJ, Sheahan D, Desbrow C, Brighty GC, Waldock M, Sumpter JP. 1998. Identification of estrogenic chemicals in STW effluent. 2. In vivo responses in trout and roach. Environ Sci Technol 32: 1559-1565.
Sanderson H, Johnson DJ, Wilson CJ, Brain RA, Solomon KR. 2003. Probabilistic hazard assessment of environmentally occurring pharmaceuticals toxicity to fish, daphnids and algae by ECOSAR screening. Toxicol Lett 144: 383-395.
Sarakinos HC, Bermingham N, White PA, Rasmusssen JB. 2000. Correspondence between whole effluent toxicity and the presence of priority substances in complex industrial effluents. Environ Toxicol Chem 19: 63-71.
Schirling M, Bohlen A, Triebskorn R, Köhler H-R. 2006. An invertebrate embryo test with the apple snail Marisa cornuarietis to assess effects of potential developmental and endocrine disruptors. Chemosphere 64: 1730-1738.
Schowanek D, Webb S. 2002. Exposure simulation for pharmaceuticals in European surface waters with GREAT-ER. Toxicol Lett 131: 39-50.
Schultz IR, Orner G, Merdink JL, Skillman A. 2001. Dose-response relationships and pharmacokinetics of vitellogenin in rainbow trout after intravascular administration of 17α-ethynylestradiol. Aquat Toxicol 51: 305-318.
Schwaiger J, Spieser OH, Bauer C, Ferling H, Mallow U, Kalbfus W, Negel RD. 2000. Chronic toxicity of nonylphenol and ethinylestradiol: haematological and histopathological effects in juvenile common carp (*Cyprinus carpio*). Aquat Toxicol 51: 69-78.
Segers JHL, Temmink JHM, van den Berg JHJ, Wegman RCC. 1984. Morphological changes in the gill of carp (*Cyprinus carpio* L.) exposed to acutely toxic concentrations of methyl bromide. Water Res 18: 1437-1441.
Sheahan DA, Bucke D, Matthiessen P, Sumpter JP, Kirby MF, Neall P, Waldock M. The effects of low leves of 17α-ethynylestradiol upon plasma vitellogenin levels in male and female rainbow trout, *Oncorhynchus mykiss* held at two acclimation temperatures. In: Lloyd R, ed. Sublethal and chronic effects of pollutants on freshwater fish.
Sills McMurry C, Dickerson RL. 2001. Effects of binary mixtures of six xenobiotics on hormone concentrations and morphometric endpoints of northern bobwhite quail (*Colinus virginianus*). Chemosphere 43: 829-837.
Stanton JM, Fisher JM. 1985. Growth of Wheat after Damage by, and Effects of Ethylene Dibromide on, a Field Population of *Heterodero avenae*. Aust J Agric Res 36: 559-568.
Steinberg CEW, Sturm A, Kelbel J, Kyu Lee S, 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.
Straub JO. 2002. Environmental risk assessment for new human pharmaceuticals in the European

Union according to the draft guideline/discussion paper of January 2001. Toxicol Lett 135: 231-237.
Strong RG, Lindgren DL. 1959. Effect of Methyl Bromide and Hydrocyanic Acid Fumigation on the Germination of Wheat. J Econ Entomol 52: 51-60.
Strong RG, Lindgren DL. 1961. Effect of Methyl Bromide and Hydrocyanic Acid Fumigation on the Germination of Corn Seed. J Econ Entomol 54: 764-770.
Sun B, Nirmalakhandan N, Hall E, Wang XH, Prakash J, Maynes R. 1994. Estimating Toxicity of Organic Chemicals to Activated-Sludge Microorganisms. J Environ Eng 120: 1459-1469.
Ternes TA, Kreckel P, Mueller J. 1999. Behaviour and occurence of estrogens in municipal sewage treatment plants - II. Aerobic batch experiments with activated sludge. Sci Total Environ 225: 91-99.
Tiedge H, Nagel R, Urich K. 1986. Effect of Substituted Phenols on Transaminase Activity in the Fish, *Leuciscus idus melanotus* L. Bull Environ Contam Toxicol 36: 176-180.
Trevizo C, Nirmalakhandan N. 1999. Prediction of Microbial Toxicity of Industrial Organic Chemicals. Water Sci Technol 39: 63-69.
US EPA. 2003. Summaries. 793-24-8. 1,4-Benzenediamine, N-(1,3-dimethylbutyl)-N'-phenyl-. US EPA, website High Production Volume Challange Program: US EPA. 34 pp.
Van den Belt K, Berckmans P, Vangenechten C, Verheyen R, Witters H. 2004. Comparative study on the in vitro/in vivo estrogenic potencies of 17β-estradiol, estrone, 17α-ethynylestradiol and nonylphenol. Aquat Toxicol 66: 183-195.
Van den Belt K, Wester PW, Van der Ven LTM, Verheyen R, Witters H. 2002. Effects of ethinylestradiol on the reproductive physiology in zebrafish (*Danio rerio*): time dependency and reversibility. Environ Toxicol Chem 21: 767-775.
Van Gundy SD, Munnecke D, Bricker J, Minteer R. 1972. Response of Meloidogyne incognita, Xiphinema index, and Dorylaimus sp. to Methyl Bromide Fumigation. Phytopathol 62: 191-192.
Van Straalen NM, Van Gestel CAM. 1999. Ecotoxicological risk assessment of pesticides subject to long-range transport. Water, Air, Soil Pollut 115: 71-81.
Vanachter A. 1974. Soil disinfestation in cauliflower, tomato and witloof crops in Belgium. Agric Environ 1: 265-276.
Vandenbergh GF, Adriaens D, Verslycke T, Janssen CR. 2003. Effects of 17α-ethinylestradiol on sexual development of the amphipod *Hyalella azteca*. Ecotoxicol Environ Saf 54: 216-222.
Verschaeve L, van Gompel J, Thilemans L, Regniers L, Vanparys P, van der Lelie D. 1999. VITOTOX® bacterial genotoxicity and toxicity test for the rapid sceening of chemicals. Environ Mol Mutagen 33: 240-248.
Wade NL, Rigney CJ. 1979. Phytotoxicity of Ethylene Dibromide to Cherry and Banana Fruit. J Am Soc Hortic Sci 104: 900-903.
Walker WW, Hawkins WE, Heard CS, Overstreet RM. 1998. Toxic, Carcinogenic and Hepatic Biochemical Effects of Ethylene Dibromide on the Japanese Medaka (*Oryzias latipes*). 454.
Watts MM, Pascoe D, Carrol K. 2001. Chronic effects to 17alpha-ethinylestradiol and bisphenol A - effects on development and reproduction in the freshwater invertebrate *Chironomus riparius* (Diptera: Chironomidae). Aquat Toxicol 55: 113-124.
Watts MM, Pascoe D, Carrol K. 2002. Population responses of the freswater amphipod *Gammarus pulex* (L.) to an environmental estrogen, 17α-ethinylestradiol. Environ Toxicol Chem 21: 445-450.
Weber LP, Balch GC, Metcalfe CD, Janz DM. 2004. Increased kidney, liver, and testicular cell death after chronic exposure to 17α-ethinylestradiol in medaka (*Oryzias latipes*). Environ Toxicol Chem 23: 792-797.
Wegman RCC, Greve PA. 1981. Methyl Bromide and Bromide-Ion in drainage water after leaching of glasshouse soils. Water, Air, Soil Pollut 16: 3-11.

Weihing JL, Schuster ML, Riesselman JH, Cook JA. 1971. Control of Fusarium wilt of Petunia with three soil fumigants. Plant Dis Rep 55: 580-582.

Wellens H. 1982. Vergleich der Empfindlichkeit von Brachydanio rerio und Leuciscus idus bei der Untersuchung der Fischtoxizität von chemischen Verbindungen und Abwässern. Zeitschrift für Wasser-Abwasser-Forschung 15: 49-52.

Weller GL, Van S.Graver JE. 1998. Cut flower disinfestation: Assessment of replacement fumigants for methyl bromide. Postharvest Biol Tec 14: 325-333.

Wells JM, Payne JA. 1975. Mycoflora of Pecans Treated with Heat, Low Temparatures, or Methyl Bromide for Control of the Pecan Weevil. Phytopathol 65: 1393-1395.

Wester PW, Canton JH, Dormans JAMA. 1988. Pathological effects in freshwater fish *Poecilia reticulata* (guppy) and *Oryzias latipes* (medaka) following methyl bromide and sodium bromide exposure. Aquat Toxicol 12: 323-344.

Weststeijn G. 1973. Soil sterilization and glasshouse disinfection to control Fusarium oxysporum f. lycopersici in tomatoes in the Netherlands. Neth J Plant Path 79: 36-40.

Wilhelm S. 1966. Chemical treatments and inoculum potential of soil. Annu Rev Phytopathol 4: 53-78.

Yang RSH, Witt KL, Alden CJ, Cockerham LG. 1995. Toxicology of Methyl Bromide. Rev Environ Contam Toxicol 142: 65-85.