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Environmental Risk Limits for alcohols, glycols, and some other relatively soluble and/or volatile compounds

1. Ecotoxicological evaluation

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Rapport in het kort

Milieurisicogrenzen voor alcoholen, glycolen en enkele andere relatief oplosbare en/of vluchtige verbindingen 1. Ecotoxicologische evaluatie

In dit rapport zijn maximaal toelaatbaar risiconiveaus (MTR), verwaarloosbaar risiconiveaus (VR) en ernstig risiconiveaus (ER_{eco}, Engelse afkorting SRC_{eco}) afgeleid voor 1-butanol, 2-butanol, *n*-butylacetaat, cyclohexylamine, diethyleenglycol, ethyleenglycol, ethylacetaat, methanol, methylethylketon, tribroommethaan en triethanolamine. Deze milieurisicogrenzen zijn afgeleid voor de compartimenten water, bodem en sediment en zijn gebaseerd op milieuchemische gegevens en ecotoxicologische gegevens voor met name het aquatische milieu. De risiconiveaus vormen de basis voor een schatting van het potentiële risico van stoffen voor een ecosysteem. Dit rapport heeft een bijbehorend deel van Traas en Bontje, gepubliceerd in 2005, waarin het blootstellingsmodel Humanex wordt gebruikt om MTRs voor de mens te berekenen, met als doel om milieurisicogrenzen af te leiden, die beschermend zijn voor zowel de mens als ecosystemen.

Trefwoorden: milieurisicogrenzen; alcoholen, glycolen, maximaal toelaatbaar risiconiveau, verwaarloosbaar risiconiveau, ernstig risiconiveau

Abstract

Environmental Risk Limits for alcohols, glycols, and some other relatively soluble and/or volatile compounds 1. Ecotoxicological evaluation

In this report, maximum permissible concentrations (MPC), negligible concentrations (NC) and serious risk concentrations (SRC_{eco}) are derived for the following compounds: 1-butanol, 2-butanol, *n*-butyl acetate, cyclohexylamine, diethylene glycol, ethyl acetate, ethylene glycol, methanol, methyl ethyl ketone, tribromomethane and triethanolamine. These environmental risk limits are derived for the water, soil and sediment compartments and are based on environmental chemistry data and data on ecotoxicology, mainly for the aquatic environment. These risk limits serve as the basis for an estimation of the potential risks of substances to an ecosystem. This report has a companion report by Traas and Bontje, published in 2005, in which the exposure model Humanex is used to calculate maximum permissible concentrations for humans, to derive risk limits that protect both humans and ecosystems.

Keywords: environmental risk limits, alcohols, glycols, maximum permissible concentration, negligible concentration, serious risk concentration

Contents

Samenvatting

Milieurisicogrenzen vormen het uitgangspunt voor een schatting van het potentiële risico van stoffen voor ecosystemen en worden afgeleid met gebruik van ecotoxicologische en milieuchemische gegevens. Milieurisicogrenzen dienen als de wetenschappelijke basis voor milieukwaliteitsnormen die worden vastgesteld door de Stuurgroep Stoffen. In dit rapport zijn de milieurisicogrenzen ernstig risiconiveau voor ecosystemen (ER_{eco}; Engelse afkorting SRC_{eco}), maximaal toelaatbaar risiconiveau (MTR) en verwaarloosbaar risiconiveau (VR) afgeleid voor een heterogene groep van verbindingen. Deze groep van elf stoffen bestaat uit een aantal vrij vluchtige verbindingen, die gebruikt worden als oplosmiddelen (1-butanol, 2-butanol, *n*-butylacetaat, ethylacetaat, methanol, methylethylketon en tribroommethaan), als antivriesvloeistoffen (ethyleenglycol en diethyleenglycol), als ingrediënt van wasmiddelen (triethanolamine) en als emulgator (cyclohexylamine). Deze stoffen worden ook geëvalueerd met betrekking tot humane risico's, waarover apart wordt gerapporteerd (deel 2). In dat rapport worden de hier afgeleide risicogrenzen vergeleken met risicogrenzen voor de mens berekend met het blootstellingsmodel Humanex (Traas en Bontje, 2005).

Negen van de elf stoffen die in dit rapport behandeld zijn, zijn eerder geëvalueerd, bij de afleiding van de destijds geheten ecotoxicologisch ernstige bodemverontreinigings-concentraties, het huidige $ER_{eco.}$ Voor deze stoffen zijn de toxiciteitsgegevens gebruikt uit de rapporten van Crommentuijn *et al*. (1995) en Posthumus *et al*. (1998), aangevuld met recente toxiciteitsgegevens. Naast het ER_{eco} werden voor deze stoffen nu ook het MTR en VR afgeleid. De stoffen cyclohexylamine en triethanolamine zijn niet eerder geëvalueerd en worden in dit rapport voor het eerst behandeld.

Voor het afleiden van het MTR en het ER_{eco} voor water werd in alle gevallen gebruik gemaakt van veiligheidsfactoren volgens de leidraad van de EU voor de risicobeoordeling van nieuwe stoffen, bestaande stoffen en biociden (TGD). Voor bodem- en sedimentorganismen zijn vrijwel geen toxiciteitsgegevens gevonden. Derhalve zijn de MTR- en ER_{eco}-waarden voor de compartimenten bodem en sediment voor de elf stoffen afgeleid met behulp van de evenwichtspartitiemethode volgens de TGD. Voor een overzicht van de afgeleide milieurisicogrenzen, zie tabel 1 tot en met 4.

Tabel 1. Overzicht van VR-, MTR- en ER_{eco}-waarden voor zoetwater. Normen voor totaal en opgeloste concentraties zijn gelijk.

Stof	VR [mg/L]	MTR [mg/L]	ER_{eco} [mg/L]
1-butanol	0,0022	0,22	94
2-butanol	0,0095	0,95	310
n-butylacetaat	$1,8 \cdot 10^{-4}$	0,018	9,4
cyclohexylamine	$2,0 \cdot 10^{-6}$	$2,0 \cdot 10^{-4}$	1,2
diethyleenglycol	0,15	15	4100
ethylacetaat	0,0011	0,11	66
ethyleenglycol	2,0	200	2900
methanol	0,0019	0,19	1200
methylethylketon	0,012	1,2	410
tribroommethaan	$9,6 \cdot 10^{-4}$	0,096	4,1
triethanolamine	0,0032	0,32	82

Tabel 2. Overzicht van VR-, MTR- en ER$_{eco}$-waarden voor zeewater. Normen voor het totaal en opgeloste concentraties zijn gelijk.

Stof	VR [mg/L]	MTR [mg/L]	ER$_{eco}$ [mg/L]
1-butanol	0,0021	0,21	94
2-butanol	$9{,}5\cdot10^{-4}$	0,095	310
n-butylacetaat	$1{,}8\cdot10^{-5}$	0,0018	9,4
cyclohexylamine	$2{,}0\cdot10^{-7}$	$2{,}0\cdot10^{-5}$	1,2
diethyleenglycol	0,015	1,5	4100
ethylacetaat	$1{,}1\cdot10^{-4}$	0,011	66
ethyleenglycol	0,20	20	6800
methanol	$1{,}9\cdot10^{-4}$	0,019	1200
methylethylketon	0,0012	0,12	410
tribroommethaan	$1{,}5\cdot10^{-5}$	0,0015	1,0
triethanolamine	$3{,}2\cdot10^{-4}$	0,032	82

Tabel 3. Overzicht van VR-, MTR- en ER$_{eco}$-waarden voor standaardbodem (10 % organisch materiaal en 25 % klei).

Stof	VR [mg/kg$_{dw}$]	MTR [mg/kg$_{dw}$]	ER$_{eco}$ [mg/kg$_{dw}$]
1-butanol	0,0015	0,15	63
2-butanol	0,0068	0,68	220
n-butylacetaat	$9{,}6\cdot10^{-4}$	0,096	50
cyclohexylamine	$8{,}1\cdot10^{-6}$	$8{,}1\cdot10^{-4}$	5,0
diethyleenglycol	0,066	6,6	1800
ethylacetaat	0,0020	0,20	130
ethyleenglycol	0,89	89	1300
methanol	$9{,}8\cdot10^{-4}$	0,098	630
methylethylketon	0,022	2,2	750
tribroommethaan	0,011	1,1	46
triethanolamine	0,0019	0,19	47

Tabel 4. Overzicht van VR-, MTR- en ER$_{eco}$-waarden voor standaardsediment (10 % organisch materiaal en 25 % klei).

Stof	VR [mg/kg$_{dw}$]	MTR [mg/kg$_{dw}$]	ER$_{eco}$ [mg/kg$_{dw}$]
1-butanol	0,0054	0,54	230
2-butanol	0,023	2,3	770
n-butylacetaat	0,0013	0,13	66
cyclohexylamine	$1{,}2\cdot10^{-5}$	0,0012	7,2
diethyleenglycol	0,32	32	8900
ethylacetaat	0,0039	0,39	240
ethyleenglycol	4,3	430	6200
methanol	0,0043	0,43	2700
methylethylketon	0,043	4,3	1500
tribroommethaan	0,012	1,2	53
triethanolamine	0,0074	0,74	190

Summary

Environmental risk limits (ERLs) are a starting point for an estimation of the potential risks of substances to ecosystems and are derived from data on environmental chemistry and on ecotoxicological data. ERLs serve as the scientific basis for Environmental Quality Standards set by the Steering Committee for Substances, and are derived using data on (eco)toxicology and environmental chemistry. In this report, the ERLs serious risk concentration for ecosystems (SRC_{eco}), maximum permissible concentration (MPC), and negligible concentration (NC) are derived for a heterogeneous group of eleven compounds, used as organic solvents (1-butanol, 2-butanol, *n*-butyl acetate, ethyl acetate, methanol, methyl ethyl ketone and tribromomethane), as surfactant in detergents (triethanolamine), as antifreeze fluids (ethylene glycol and diethylene glycol), and as emulsifier (cyclohexylamine). The same compounds will also be evaluated for human risk limits in the context of background levels in a separate report (part 2). In that report, the risk limits derived here are compared with risk limits for humans calculated by the exposure model Humanex (Traas and Bontje, 2005).

Among the eleven compounds considered in this report, nine have already been evaluated in the context of deriving ecotoxicological Serious Risk Concentrations (SRC_{eco}). For these compounds existing ecotoxicological data reported in Crommentuijn *et al*. (1995) and Posthumus *et al*. (1998) are used together with new data that have become available since then. For these compounds the MPC and NC values were now derived as well as the SRC_{eco}. Cyclohexylamine and triethanolamine have not been evaluated before and the first data search and ERL derivation for both compounds are reported in the present document.

For the water compartment, MPC and SRC_{eco} values are derived using assessment factors according to the EU technical guidance for the risk assessment of new and existing substances and biocides (TGD). For the sediment and soil inhabiting organisms, no toxicity data were available. Therefore, SRC_{eco} and MPC values for the soil and sediment compartment were derived using equilibrium partitioning theory, according to the methodology of the TGD. For an overview of the ERLs derived in this report, see Table 1 to 4.

Table 1. Overview of NC, MPC, and SRC_{eco} values for freshwater. Values for total and dissolved concentrations are equal.

Compound	NC [mg/L]	MPC [mg/L]	SRC_{eco} [mg/L]
1-butanol	0.0022	0.22	94
2-butanol	0.0095	0.95	310
n-butyl acetate	$1.8 \cdot 10^{-4}$	0.018	9.4
cyclohexylamine	$2.0 \cdot 10^{-6}$	$2.0 \cdot 10^{-4}$	1.2
diethylene glycol	0.15	15	4100
ethyl acetate	0.0011	0.11	66
ethylene glycol	2.0	200	2900
methanol	0.0019	0.19	1200
methyl ethyl ketone	0.012	1.2	410
tribromomethane	$9.6 \cdot 10^{-4}$	0.096	4.1
triethanolamine	0.0032	0.32	82

Table 2. Overview of NC, MPC, and SRC_{eco} values for seawater. Values for total and dissolved fraction are equal.

Compound	NC [mg/L]	MPC [mg/L]	SRC_{eco} [mg/L]
1-butanol	0.0021	0.21	94
2-butanol	$9.5 \cdot 10^{-4}$	0.095	310
n-butyl acetate	$1.8 \cdot 10^{-5}$	0.0018	9.4
cyclohexylamine	$2.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-5}$	1.2
diethylene glycol	0.015	1.5	4100
ethyl acetate	$1.1 \cdot 10^{-4}$	0.011	66
ethylene glycol	0.20	20	6800
methanol	$1.9 \cdot 10^{-4}$	0.019	1200
methyl ethyl ketone	0.0012	0.12	410
tribromomethane	$1.5 \cdot 10^{-5}$	0.0015	1.0
triethanolamine	$3.2 \cdot 10^{-4}$	0.032	82

Table 3. Overview of NC, MPC and SRC_{eco} values for standard soil (Dutch standard soil, containing 10 % organic matter and 25 % clay).

Compound	NC [mg/kg_{dw}]	MPC [mg/kg_{dw}]	SRC_{eco} [mg/kg_{dw}]
1-butanol	0.0015	0.15	63
2-butanol	0.0068	0.68	220
n-butyl acetate	$9.6 \cdot 10^{-4}$	0.096	50
cyclohexylamine	$8.1 \cdot 10^{-6}$	$8.1 \cdot 10^{-4}$	5.0
diethylene glycol	0.066	6.6	1800
ethyl acetate	0.0020	0.20	130
ethylene glycol	0.89	89	1300
methanol	$9.8 \cdot 10^{-4}$	0.098	630
methyl ethyl ketone	0.022	2.2	750
tribromomethane	0.011	1.1	46
triethanolamine	0.0019	0.19	47

Table 4. Overview of NC, MPC and SRC_{eco} values for standard sediment (Dutch standard sediment, containing 10 % organic matter and 25 % clay).

Compound	NC [mg/kg_{dw}]	MPC [mg/kg_{dw}]	SRC_{eco} [mg/kg_{dw}]
1-butanol	0.0054	0.54	230
2-butanol	0.023	2.3	770
n-butyl acetate	0.0013	0.13	66
cyclohexylamine	$1.2 \cdot 10^{-5}$	0.0012	7.2
diethylene glycol	0.32	32	8900
ethyl acetate	0.0039	0.39	240
ethylene glycol	4.3	430	6200
methanol	0.0043	0.43	2700
methyl ethyl ketone	0.043	4.3	1500
tribromomethane	0.012	1.2	53
triethanolamine	0.0074	0.74	190

1. Introduction

This report is part of the project 'International and National Environmental Quality Standards for Substances in the Netherlands'. The aim of the project is to derive environmental risk limits (ERLs) for substances in the environment for the compartments air, (ground)water, sediment and soil. Environmental risk limits (ERLs) serve as advisory values to set environmental quality standards (EQS) by the Steering Committee for Substances for various policy purposes. The term EQS is used to designate all legally and non-legally binding standards that are used in Dutch environmental policy and Table 5 shows the correspondence between ERLs and EQSs. The various ERLs are:

- the Negligible Concentration (NC) for water, soil, groundwater, sediment and air;
- the Maximum Permissible Concentration (MPC) for water, soil, groundwater sediment and air;
- the ecotoxicological Serious Risk Concentration for water, soil, groundwater and sediment (SRC_{eco}).

Table 5. Environmental risk limits (ERLs) and the related environmental quality standards (EQS) that are set by the Dutch government in the Netherlands for the protection of ecosystems.

Description	ERL	EQS
The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects.	NC (for air, water, soil, groundwater and sediment)	Target value (for air, water, soil, groundwater and sediment)
The MPC is the concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the hazardous concentration for 5% of the species, the $HC5_{NOEC}$.	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water and sediment)
The SRC_{eco} is the concentration of a substance in the soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected, the $HC50_{NOEC}$.	SRC_{eco} (for water, soil, groundwater and sediment)	Intervention value after comparison with SRC_{human} (for soil, sediment and groundwater)

The process of deriving ERLs is shown schematically in Figure 1. ERLs for soil and sediment are calculated for a standardised soil. ERLs for water are reported for dissolved and total concentrations (including a standard amount of suspended matter) and if found significantly different, differentiated to freshwater and saltwater. Each of the ERLs and its corresponding EQS represents a different level of protection, with increasing numerical values in the order Target Value < MPC[1] < Intervention Value. The EQS demand different actions when one of them is exceeded, explained elsewhere (VROM, 2001).
In the series of RIVM reports that were published in the framework of the project 'Setting Integrated Environmental Quality Standards', (now called 'International and National

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[1] A complicating factor is that the term MPC is used both as an ERL and as an EQS. For historical reasons, however, the same term is used.

Environmental Quality Standards for Substances in the Netherlands'), ERLs were derived for approximately 250 substances and groups of substances. For an overview of the EQSs set by the Ministry of VROM, see VROM (2001). The Expert Centre for Substances of RIVM has recently launched a website at which all EQSs are available. The web site can be found at: http://www.stoffen-risico.nl.

In this report, ERLs are derived for a group of compounds. The results obtained until now in the project 'International and National Environmental quality standards for Substances in the Netherlands' are laid down in several reports. In this project the ERLs are derived according to the Technical Guidance Document (TGD), issued by the European Commission and developed in support of the risk assessment of new notified chemical substances, existing substances and biocides (European Commission, 2003). The SRC_{eco}s for 8 out of the 11 compounds were already derived (Table 6) and reported by Crommentuijn *et al*. (1995) and Posthumus *et al*. (1998). In these reports, no MPC values were derived. In the present report, toxicity data were updated and MPCs, NCs and revised SRC_{eco} values are calculated. In a second phase of the project, risk limits were calculated that also protect humans and these were compared to ecotoxicological risk limits. This report also contains the scientific advisory values that protect both humans and ecosystems (Traas and Bontje, 2005).

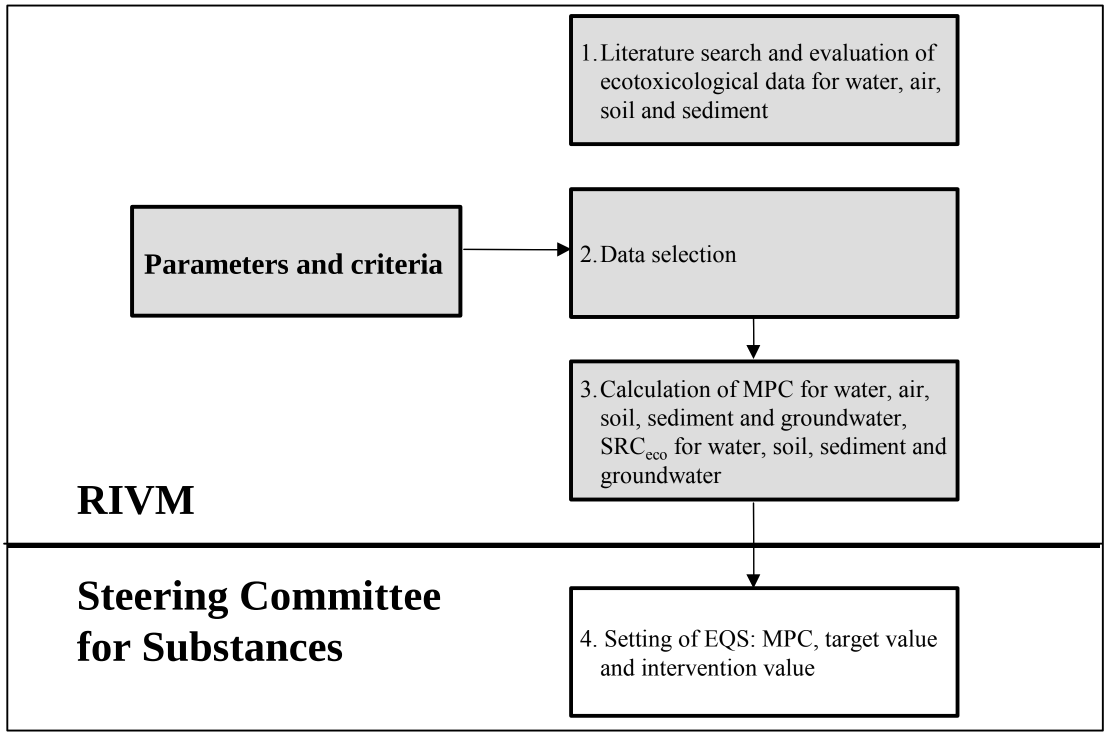


Figure 1. The process of deriving Environmental Risk Limits. Above the line the method to derive ERLs is indicated, i.e. MPC, NC and SRC_{eco}. Below the dashed line the MPC, Target Value and Intervention Value is indicated, set by the Steering Committee for Substances.

Table 6. List of compounds treated in this report and references of previous reports where underlying data can be found.

Compounds	References or/and new data	Previously derived ERLs
butanol (1- and 2-butanol)	Crommentuijn *et al*., 1995 (1-butanol); new data	SRC_s
n-butyl acetate	Posthumus *et al*., 1998; Crommentuijn *et al*., 1995; new data	SRC_s SRC_s
cyclohexylamine	new data	-
diethylene glycol	Crommentuijn *et al*., 1995; new data	SRC_s
ethyl acetate	Posthumus *et al*., 1998; new data	SRC_s
ethylene glycol	Crommentuijn *et al*., 1995; new data	SRC_s
methanol	Crommentuijn *et al*., 1995; new data	SRC_s
methyl ethyl ketone (MEK)	Crommentuijn *et al*., 1995; new data	SRC_s
tribromomethane (bromoform)	Posthumus *et al*., 1998; new data	SRC_s
triethanolamine	new data	-

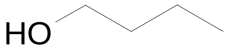
2. Substance properties and use

2.1 Physicochemical properties

Table 7. General information and physicochemical properties of 1-butanol. Bold values indicate preferential values used in calculations.

1-butanol

CASnr. 71-36-3

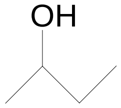


Property	Value	Reference
Water solubility [mg/L]	73100	shake flask-cloud point, Butler *et al*., 1993
	73320	shake flask-residue volume, Booth & Everson, 1948
	74100	shake flask-interferometry, Hansen *et al*., 1949
	77800	shake flask-GC, Korenman *et al*., 1974, 1975
	74000	shake flask colorimetric analysis, De Santis *et al*.., 1976
	78100	shake flask-GC, Doucette & Andren, 1988
	65720	shake flask-GC, Li *et al*., 1992
	73633	**Geometric mean**
Log K_{ow}	0.93	shake flask-RC, Cornford, 1982
	0.79	generator column GC, Wasik *et al*., 1981
	0.87	shake flask-GC, Riebesehl & Tomlinson, 1986
	0.79	generator column GC, Schantz & Martire, 1987
	0.88	**MlogP**, BioByte, 2004; Hansch & Leo, 1985
Log K_{oc}	0.50	Sabljić *et al*., 1995; Meylan *et al*., 1992
	0.84	calculated according to Sabljić *et al*., 1995 (alcohols)
	0.67	**Average**
Henry's Law Constant $[Pa.m^3.mol^{-1}]$	0.860	Hine & Mookerjee, 1975
	0.800	Snider & Dawson, 1985
	0.892	Buttery *et al*. 1969 (SRC PhysProp), recommended value
	0.850	**Geometric mean**
Vapour pressure [Pa]	879	interpolated-regression of tabulated data, Kahlbaum, 1998
	890	extrapolated-Antoine eqn., Boublik *et al*., 1984
	904	modified isoteniscope method, Butler *et al*., 1935
	939	interpolated-regression of tabulated data, Stull, 1947
	936	experimental, Daubert & Danner, 1985
	914	**Geometric mean**

Table 8. General information and physicochemical properties of 2-butanol. Bold values indicate preferential values used in calculations.

2-butanol

CASnr. 78-92-2

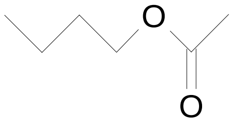


Property	Value	Reference
Water solubility [mg/L]	**181000**	experimental, Hefter, 1984 (from SRC PhysProp Database)
Log K_{ow}	**0.61**	**MlogP**, BioByte, 2004; Hansch & Anderson, 1967
Log K_{oc}	**0.74**	calculated according to Sabljić *et al*., 1995 (alcohols)
Henry's Law Constant $[Pa.m^3.mol^{-1}]$	1.040	partial pressure-isoteniscope, Butler, 1935
	0.800	headspace-GC, Snider & Dawson, 1985
	0.912	**Geometric mean**
Vapour pressure [Pa]	2286	modified isoteniscope method, Butler *et al*., 1935
	2266	interpolated-regression of tabulated data, Stull, 1947
	2440	measured, Banerjee *et al*., 1990
	2329	**Geometric mean**

Table 9. General information and physicochemical properties of n-*butyl acetate. Bold values indicate preferential values used in calculations.*

***n*-butyl acetate**

CASnr. 123-86-4

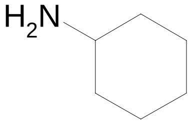


Property	Value	Reference
Water solubility [mg/L]	23580	shake flask-AS, Hansch *et al*., 1968
	6702	gen. col.-GC, Wasik *et al*., 1981, 1982
	8400	experimental, Yalkowsky & Dannenfelser, 1992 (from SRC PhysProp Database)
	6290	experimental, Syracuse Research Crop, 1979 (SRC Chemfate)
	9559	**Geometric mean**
Log K_{ow}	1.82	gen. col.-GC, Wasik *et al*., 1981, 1982; Tewari *et al*., 1982; Howard, 1990
	1.78	**MlogP**, BioByte, 2004
Log K_{oc}	**1.92**	calculated according to Sabljić *et al*., 1995 (esters)
Henry's Law Constant [Pa.m^3.mol^{-1}]	**28.51**	Vapour-liquid equilibrium, vapour phase-GC, Kiekbusch & King, 1979
Vapour pressure [Pa]	1530	extrapolated-Antoine eqn., Boublik *et al*., 1984
	1529	extrapolated-Antoine eqn., Dean, 1985
	2000	measured, Banerjee *et al*., 1990
	1673	**Geometric mean**

Table 10. General information and physicochemical properties of cyclohexylamine. Bold values indicate preferential values used in calculations.

cyclohexylamine

CASnr. 108-91-8

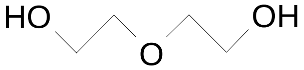


Property	Value	Reference
Water solubility [mg/L]	**1000 000 (20 °C)**	experimental, Merck Index, 1996 (from SRC PhysProp Database)
pK_a	10.66	Mackay *et al*., 2000
	10.68	BioByte, 2004
Log K_{ow}	**1.49**	**MlogP**, BioByte, 2004**;** Hansch *et al*., 1995
Log K_{oc}	**1.79**	calculated according to Sabljić *et al*., 1995 (nonhydrophobics)
Henry's Law Constant [Pa.m^3.mol^{-1}]	**0.421**	experimental, Altschuh *et al*., 1999 (from SRC PhysProp Database)
Vapour pressure [Pa]	**1346**	experimental, Daubert & Danner, 1989 (from SRC PhysProp Database)

Table 11. General information and physicochemical properties of diethylene glycol. Bold values indicate preferential values used in calculations.

diethylene glycol

CASnr. 111-46-6

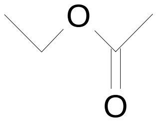


Property	Value	Reference
Water solubility [mg/L]	**1000 000**	experimental, Riddick *et al*., 1986 (from SRC PhysProp Database)
Log K_{ow}	**-1.30**	**ClogP**, calculated, BioByte, 2004
Log K_{oc}	**-0.01**	calculated according to Sabljić *et al*., 1995 (alcohols)
Henry's Law Constant [Pa.m^3.mol^{-1}]	**0.000203**	estimated, Meylan & Howard, 1991 (from SRC PhysProp Database)
Vapour pressure [Pa]	0.76	experimental, Daubert & Danner, 1991 (from SRC PhysProp Database)
	1.04	experimental, Daubert & Danner, 1989 (SRC Chemfate)
	0.89	**Geometric mean**

Table 12. General information and physicochemical properties of ethyl acetate. Bold values indicate preferential values used in calculations.

ethyl acetate

CASnr. 141-78-6

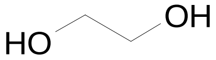


Property	Value	Reference
Water solubility [mg/L]	80350	shake flask-AS, Hansch *et al*., 1968
	80000	shake flask-HPLC, Banerjee, 1984
	78720	shake flask-centrifuge, Booth & Everson, 1948
	79780	shake flask-interferometry, Donahue & Bartell, 1952
	79710	**Geometric mean**
Log K_{ow}	0.73	shake flask-GC, Hansch & Anderson, 1967
	0.73	shake flask-UV, Hansch *et al*., 1968
	0.70	experimental, Valvani *et al*., 1981
	0.66	shake flask-CR, Collander, 1951
	0.73	**MlogP**, BioByte, 2004
Log K_{oc}	**1.41**	calculated according to Sabljić *et al*., 1995 (esters)
Henry's Law Constant [Pa.m^3.mol^{-1}]	13.42	partial pressure, Butler & Ramchandani, 1935
	17.2	vapour-liquid equilibrium, vapour phase-GC, Kiekbusch & King, 1979
	15.2	**Geometric mean**
Vapour pressure [Pa]	11860	interpolated-regression of tabulated data, Stull, 1947
	12600	ebulliometry, fitted to Antoine eqn., Ambrose *et al*., 1981
	3240	measured, Banerjee *et al*., 1990
	12424	experimental, Daubert & Danner, 1991 (from SRC PhysProp Database)
	8807	**Geometric mean**

Table 13. General information and physicochemical properties of ethylene glycol. Bold values indicate preferential values used in calculations.

ethylene glycol (1,2-ethanediol)

CASnr. 107-21-1



Property	Value	Reference
Water solubility [mg/L]	**miscible/infinite**	Dean, 1985, Riddick *et al*., 1986, Yaws *et al*., 1990
Log K_{ow}	-0.54	shake flask-CR, Collander, 1951
	-1.36	**MlogP**, BioByte, 2004, Hansch & Leo, 1985
Log K_{oc}	**-0.03**	calculated according to Sabljić *et al*., 1995 (alcohols)
Henry's Law Constant [Pa.m^3.mol^{-1}]	**0.00608**	experimental, Butler & Ramchandani, 1935 (from SRC PhysProp Database)
Vapour pressure [Pa]	11.70	ebulliometry, extrapolated-Antoine eqn., Ambrose & Hall, 1981
	9.299	extrapolated-Antoine eqn., Boublik *et al*., 1984
	11.86	extrapolated-Antoine eqn., Dean, 1985
	12.26	experimental, Daubert & Danner, 1985 (from SRC PhysProp Database)
	11.22	**Geometric mean**

Table 14. General information and physicochemical properties of methanol. Bold values indicate preferential values used in calculations.

methanol

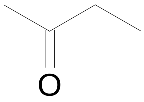
CASnr. 67-56-1

$H_3C—OH$

Property	Value	Reference
Water solubility [mg/L]	**Miscible**	**Dean, 1985; Howard, 1990; Pinal *et al.*, 1991; Yaws *et al.*, 1990**
log K_{ow}	-0.66	shake flask-GC, Hansch & Anderson, 1967
	-0.77	shake flask-GC, Leo *et al*., 1975
	-0.52	shake flask-RC, Cornford, 1982
	-0.77	**MlogP**, BioByte, 2004
log K_{oc}	0.44	quoted, experimental, Meylan *et al*., 1992
	0.20	calculated according to Sabljić *et al*., 1995 (alcohols)
	0.32	**Average**
Henry's Law Constant [Pa.m^3.mol^{-1}]	0.444	entrainment method-GC, Burnett, 1963
	0.450	headspace-GC, Snider & Dawson, 1985
	0.461	experimental, Gaffney *et al*., 1987 (from SRC PhysProp Database)
	0.452	**Geometric mean**
Vapour pressure [Pa]	16210	interpolated regression of tabulated data, Stull, 1947
	16958	quoted, experimental, Boublik *et al*., 1984 (from SRC PhysProp Database)
	16796	experimental, Daubert & Danner, 1989 (SRC Chemfate)
	16652	**Geometric mean**

Table 15. General information and physicochemical properties of methyl ethyl ketone. Bold values indicate preferential values used in calculations.

methyl ethyl ketone (MEK; 2-butanone)



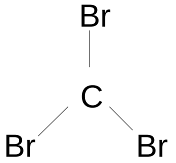
CASnr. 78-93-3

Property	Value	Reference
Water solubility [mg/L]	136280	gen. col.-GC, Wasik *et al*., 1981
	223000	experimental, Taft *et al*., 1985 (from SRC PhysProp Database)
	343550	shake flask-volumetric, Ginnings *et al*., 1940
	218562	**Geometric mean**
log K_{ow}	0.26	shake flask-CR, Collander, 1957
	0.28	shake flask-AS, Fujita *et al*., 1986
	0.29	shake flask-AS, GC, Hansch & Anderson, 1967; Hansch *et al*., 1968
	0.35	experimental, Valvani *et al*., 1981
	0.69	gen. col.-GC, Wasik *et al*., 1981
	0.26	shake flask-GC, Tanii *et al*., 1986
	0.29	**MlogP**, BioByte, 2004; Hansch *et al*., 1995
log K_{oc}	1.47	Captina silt loam, Walton *et al*., 1982
	1.53	McLaurin sandy loam, Walton *et al*., 1992
	1.17	calculated according to Sabljić *et al*., 1995 (nonhydrophobics)
	1.39	**Average**
Henry's Law Constant [Pa.m^3.mol^{-1}]	4.710	shake flask, partial vapour pressure-GC, Buttery *et al.*, 1971
	4.356	gas-stripping, Hawthorne, 1984
	5.760	headspace-GC, Snider & Dawson, 1985
	5.210	gas stripping-HPLC/UV, Zhou & Mopper, 1990
	5.13	**Geometric mean**
Vapour pressure [Pa]	12954	interpolated regression of tabulated data, Stull, 1947
	12080	ebulliometry, Ambrose *et al*., 1975
	12230	extrapolated-Antoine eqn., Boublik *et al*., 1984
	12023	extrapolated-Antoine eqn., Dean, 1985
	12316	**Geometric mean**

Table 16. General information and physicochemical properties of tribromomethane. Bold values indicate preferential values used in calculations.

tribromomethane (bromoform)

CASnr. 75-25-2

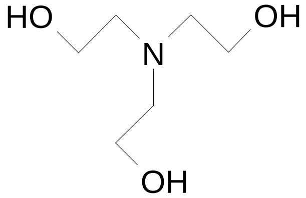


Property	Value	Reference
Water solubility [mg/L]	3100	experimental, Horvath, 1982
	3130	extrapolated between two data points, Warner *et al*., 1987
	3115	**Geometric mean**
log K_{ow}	**2.67**	**MlogP**, BioByte, 2004
log K_{oc} (L/kg)	2.06	quoted experimental, Sabljić *et al*., 1995
	2.45	Abdul *et al*., 1987 (SRC Chemfate)
	2.26	calculated according to Sabljić *et al*., 1995 (predominantly hydrophobics)
	2.26	**Average**
Henry's Law Constant [Pa.m^3.mol^{-1}]	54.2	multiple equilibration, Munz & Robert, 1987, 1989
	62.0	recommended, Mackay & Shiu, 1981, 1990
	58.0	**Geometric mean**
Vapour pressure [Pa]	720	Extrapolated data, Boublik *et al*., 1984 (from SRC PhysProp Database)
	734	Experimental, extrapolated, Daubert & Danner, 1989 (SRC Chemfate)
	727	**Geometric mean**

Table 17. General information and physicochemical properties of triethanolamine. Bold values indicate preferential values used in calculations.

triethanolamine

Casnr. 102-71-6



Property	Value	Reference
Water solubility [mg/L]	**miscible**	**Dean 1985, Riddick *et al.*, 1986**
pK_a	7.76	Mackay *et al*. 2000
	7.92	Mackay *et al*. 2000
log K_{ow}	**-1.00**	**MlogP**, BioByte, 2004; Hansch et al., 1995
log K_{oc}	**0.50**	calculated according to Sabljic & Güsten, 1995 (nonhydrophobics)
Henry's Law Constant [Pa.m^3.mol^{-1}]	**$3.42*10^{-14}$**	Hine & Mookerjee, 1975
Vapour pressure [Pa]	0.0131	extrapolated-Antoine eqn., Boublik *et al*., 1984
	0.0100	extrapolated-Antoine eqn., Dean, 1985
	0.000479	experimental, Daubert & Danner, 1989 (from SRC PhysProp Database)
	0.00856	**Geometric mean**

2.2 Properties and use

The group of compounds considered in this report deals with a heterogeneous set of 11 substances used for different goals in industries or/and in agriculture. Properties and use for each of the compounds are briefly summarised below.

2.2.1 1-Butanol

1-Butanol is a flammable colourless liquid with a rancid sweet odour. It is mainly used as a solvent for fats, waxes, resins, gums and varnishes; in the manufacture of butyl acetate, butyl acrylate, detergents, rayon and lacquers, and as diluent for brake fluids. It is used as an extractant in pharmaceutical synthesis of antibiotics, vitamins and hormones. Biodegradation in freshwater of 1-butanol is quite rapid (ranges from few hours to few days) (EHC 65, 1987).

2.2.2 2-Butanol

2-Butanol is a flammable colourless liquid with a characteristic sweet odour. 2-Butanol occurs naturally as a product of fermentation of carbohydrates. It is mainly used for the extraction of fish meal to produce fish protein concentrate, for the production of fruit essences and as a flavouring agent in food. The compound is readily biodegradable by bacteria and does not bioaccumulate (EHC 65, 1987).

2.2.3 *n*-Butyl acetate

This compound is mainly used as solvent in lacquers, artificial leathers, photographic films, plastics and safety glass (DOSE, 2000).

2.2.4 Cyclohexylamine

This compound is mainly used in organic synthesis, manufacture of plasticisers, corrosion inhibitors, rubber chemicals, dyestuffs, emulsifying agents, dry cleaning soaps, acid gas absorbants and insecticides (DOSE, 2000).

2.2.5 Diethylene glycol

This compound is a colourless liquid. It is mainly used in antifreeze solutions, as lubricant and finishing agent for wool and other fabrics, as solvent for dyestuffs and is used in composition of corks, glues, pharmaceuticals and toiletries (DOSE, 2000).

2.2.6 Ethyl acetate

Ethyl acetate is a colourless liquid with a characteristic sweet odour. It is mainly used in artificial fruit essences, as a solvent for nitrocellulose, varnishes, lacquers and in cleaning textiles and in the manufacture of photographic film, artificial silk and perfumes (DOSE, 2000).

2.2.7 Ethylene glycol

Ethylene glycol is a colourless liquid with a characteristic ether-like (sweet) odour. It is mainly used as an intermediate in the manufacture of polyethylene terephthalate (polyester); to a lesser extent as antifreeze in coolants, as an intermediate in the production of glyoxal and polyglycols, as humectant and plasticizer. The compound is readily biodegradable in aerobic and anaerobic conditions, in aquatic environment as well as in soil with sufficient moisture content. Bioaccumulation is not to be expected (GDCh, 1991).

2.2.8 Methanol

Methanol is a clear, colourless, volatile liquid with a characteristic alcoholic odour when pure. It occurs naturally in blood, urine, saliva and expired air in humans and animals. Methanol is available in the diet, principally from fresh fruit and vegetables, fruit juices, fermented beverages and diet foods. It is used in the industrial production of important compounds such as methyl *tert*-butyl ether (MTBE), formaldehyde, acetic acid, glycol methyl ethers, methylamine, methylhalides and methylmethacrylate. It is a constituent of a large number of commercially available solvents and consumer products including paints, varnishes, antifreeze solutions etc. The compound is readily degraded in the environment by photo oxidation and biodegradation processes. It is readily biodegradable under aerobic and anaerobic conditions, in a wide variety of environmental media including fresh and salt water, sediments, soils and ground water (EHC 196, 1997).

2.2.9 Methyl ethyl ketone (MEK)

Methyl ethyl ketone (MEK) is a clear, colourless, volatile, highly flammable liquid with an acetone-like odor. MEK is produced biologically and has been identified as a product of microbial metabolism. It has also been detected in higher plants, insect pheromones, animal tissues and human blood, urine and exhaled air. MEK is mainly used as a solvent in protective coatings, adhesives, paint stripper, cleaning fluid and in the manufacture of cements and as intermediate in inorganic synthesis. It is nearly completely degradable in water on the basis of biological oxygen demand (BOD) and it is not expected to accumulate in food webs (EHC 143, 1994).

2.2.10 Tribromomethane

Tribromomethane is a colourless liquid with a characteristic chloroform-like odour. The compound is mainly used as a solvent for waxes, greases and oils. It is also used as an intermediate for organic synthesis (DOSE, 2000).

2.2.11 Triethanolamine

Triethanolamine is a colourless to pale yellow viscous liquid with a slight ammoniacal odour. It is mainly used in the manufacture of detergents, cosmetics/pharmaceuticals, textile auxiliaries areas, herbicides and cement additives. The compound is considered to be inherently biodegradable at aerobic conditions in the aquatic environment. No information is available on biodegradation in soils or under anaerobic conditions (GDCh, 1994).

3. Methods

3.1 Data Search and selection

An on-line literature search was performed for the period 1985-2002. The TOXLINE and BIOSYS databases were used.

A toxicity study is considered reliable if the design of the experiment is in agreement with international accepted guidelines, e.g. OECD guidelines. Criteria are available to judge studies that have not been performed according to the OECD-guidelines, documented in Traas (2001) and the Technical Guidance Document of the EU (European Commission, 2003).

Effects on growth, reproduction or survival are used in the derivation of ERLs, as they are related to population dynamics. Toxicity data on organic substances from soil or sediment studies are normalised to 10% organic matter.

For each species and each compound, the most sensitive toxicity test is selected. If for a single species several toxicity values are found for the same effect parameter, the geometric mean is calculated.

3.2 Derivation of ERLs

3.2.1 Maximum Permissible Concentration

The maximum permissible concentrations (MPC) are derived according to the derivation of the PNEC values in the EU Technical Guidance Document (TGD) on risk assessment (European Commission, 2003, developed for EU council regulation 793/93).

In short, a data search on chronic and acute toxicity for aquatic and terrestrial species and terrestrial processes of a compound is performed. They are evaluated and selected or rejected. For the derivation of ERLs, salt and freshwater data are combined if there are no (statistical) reasons to keep the data separated. For compounds with a log K_{ow} higher than 3.0, or for compounds for which secondary poisoning is expected, toxicity data for mammals and birds are searched for as well to assess the risk of secondary poisoning. All of the compounds studied in this report have log K_{ow} values below 3 and therefore, an evaluation of secondary poisoning can be omitted.

To derive PNECs for the aquatic environment with the refined assessment method (e.g. described by Aldenberg and Jaworska, 2000), the TGD requires chronic toxicity data for at least 10 species from 8 different taxonomical groups (family, class). In the present report, this method could not be applied, because there were insufficient data for all compounds. Consequently, the maximum permissible concentration (MPC) is derived using assessment factors as laid down in the TGD.

In many cases, the only chronic toxicity data available are for unicellular organisms. According to the TGD, the results of tests with bacteria should be considered as short-term tests. Therefore, chronic tests with bacteria are not used for the derivation of the PNEC. Also chronic tests with protozoans are not used for the derivation of the PNEC, although protozoans are not explicitly mentioned in the TGD in the section on the derivation of the PNEC for aquatic organisms, but only together with bacteria in the derivation of the PNEC for sewage treatment plants (STPs).

Algae and blue-green algae (cyanophyta) are considered as primary producers according to the TGD. Chronic NOECs for these taxa should only be used in the derivation of the PNEC in combination with at least one additional NOEC for daphnids or fish. Meanwhile, the PNEC derived for any standard or non-standard organism from the acute toxicity data may not be higher than the PNEC derived from the available NOEC. Therefore, if a NOEC is available for algae or cyanophyta that is smaller than the lowest EC50 divided by 10, the MPC is based on this value.

3.2.2 Derivation of the SRCeco

The Serious Risk Concentration for ecosystems (SRC_{eco}) is derived according to the method described by Verbruggen *et al*. (2001) with some small modifications to bring the derivation of the SRC_{eco} more in line with the derivation of the MPC based on the PNEC according to the TGD. The basis for the SRC_{eco} is in principle the geometric mean of the chronic toxicity data, the hazardous concentration to 50% of the species (HC50). In the method of Verbruggen *et al*. (2001), the SRC_{eco} is equal to the geometric mean of the chronic toxicity data, if the chronic data cover at least four different taxonomical groups. In all other cases, the geometric mean of the acute data set is divided by ten and compared to the geometric mean of the chronic data. The lower of the two becomes the SRC_{eco}. However, often only unicellular organisms and mostly primary producers or consumers are represented in the chronic data, although these species belong to four taxonomical groups (algae, bacteria, cyanophyta, and protozoa). Fish or daphnids are mostly relatively sensitive species and if these species are absent in the chronic toxicity data but represented in the acute data, this may result in a geometric mean of the acute toxicity data, which is lower than of the chronic toxicity data. For this reason, a comparison between the geometric mean of the acute data set divided by ten and the geometric mean of the chronic data is always performed, unless chronic toxicity data are available for algae, *Daphnia*, and fish.

For calculating the geometric mean of the toxicity data, all species are considered, including bacteria and protozoa. When assessment factors are used to derive the PNEC, bacteria and protozoa should not be used as most sensitive species to base the PNEC upon. However, for the derivation of the geometric mean of all species, these taxa are included as well. This is in line with the application of the statistical extrapolation method according to the TGD to determine the hazardous concentration to 5% of the species (HC5) as basis for the PNEC.

3.2.3 Derivation of negligible concentrations (NCs)

The negligible concentration (NC) represents a concentration causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects such as mixture toxicity, because species are always exposed in the environment to mixtures of chemicals and complex mixtures of chemicals are generally best described as concentration-additive (Van Leeuwen *et al*., 1996; Deneer, 2000).

3.2.4 Equilibrium partitioning

If no data are available for benthic or terrestrial organisms, the MPCs for sediment and soil are calculated by equilibrium according to the TGD. In the equilibrium partitioning concept, it is assumed that equilibrium exists between the concentration of a substance sorbed to organic carbon and (pore) water. In addition, it is assumed that toxicity is related to pore water concentrations (DiToro *et al*., 1991).

The ERLs are calculated according to the TGD are for bulk (wet weight) sediment and soil. In the framework of INS, sediment and soil concentrations are normalised to dry weight, with the organic matter content of 10% for Dutch standard soil and sediment. This recalculation is performed according to the equations as documented in the guidance document for deriving Dutch Environmental Risk Limits from EU-Risk Assessment Reports (Janssen *et al*., 2004).

According to the TGD, PNECs for sediment are calculated with the characteristics of suspended matter. In this report, not only the fraction water and solids but also the organic carbon content of suspended matter is used in the recalculation of concentrations based on wet weight suspended matter to Dutch standard sediment. This results in concentrations for standard sediment, which are twice as low as calculated according to Janssen *et al.* (2004), according to which the density and composition of suspended matter must be used for the recalculation to dry weight, but at the same time the organic carbon content of sediment for the normalisation to Dutch standard sediment.

Due to the amount of a substance that is present in the (pore)water phase of sediment and soil, significant differences between the MPC for sediment and soil may occur for the non-hydrophobic compounds described in this report. This reflects the fact that although expressed as concentrations normalised to dry weight of sediment, the total amount of the substance in sediment or soil is determined by means of common extraction techniques.

For organic substances, the partition coefficient between the bulk soil/sediment (wet weight) and water is based on the organic carbon-water partition coefficient (K_{oc}), the water content of the soil and the substance contained in the air fraction. When experimental sorption coefficients (K_{oc}) are not available, these are estimated using the regression equations described by Sabljić *et al.* (1995). Experimental log K_{ow} values obtained from the MEDCHEM database (Biobyte, 2004) were used as input for the regressions. When experimental values were available, an average value between these values and the estimated value was used.

Equilibrium partitioning is also applied when the total concentration in the water phase is calculated, by calculating the contribution of the concentration of the substance in suspended solids. For the compounds considered in this report this contribution is so small, that the total concentrations in water are equal to the dissolved concentrations, for a suspended particulate matter concentration of 30 mg/L (standard value for the Netherlands).

4. Toxicity data and derivation of ERLs for water

4.1 Derivation of SRC_{eco} and MPC for water

The aquatic toxicity data that are found for 1-butanol, 2-butanol, *n*-butyl acetate, cyclohexylamine, diethylene glycol, ethyl acetate, ethylene glycol, methanol, methyl ethyl ketone, tribromomethane and triethanolamine are presented in Appendix 1, including rejected data. The selected toxicity data are given in separated tables shown below. For an overview of the derived ERLs see Table 29.

4.1.1 1-Butanol

Environmental risk limits are derived separately for 1-butanol and 2-butanol. Aquatic toxicity data for 1-butanol are given in Table A1.1. Rejected data for 1-butanol are reported in Table A1.2. The selected toxicity data for the derivation of the environmental risk limits of 1-butanol are presented in Table 18. The geometric mean of the acute freshwater toxicity data is 1233 mg/L, The geometric mean of the acute saltwater toxicity data is 2577 mg/L, and is thus twice as high. Data for freshwater and saltwater are not significantly different if a t-test with equal variance is performed on the log-transformed acute toxicity data (P=0.072). However, the variance of the toxicity data is much higher in the case of freshwater species than for saltwater species (P=0.026). The t-test with Welch-correction for unequal variance shows that are significant differences between freshwater and saltwater data (P=0.016). This is supported by the fact that for the taxa crustaceans and fish there is no overlap in toxicity data between freshwater and saltwater species, although the marine data set is too small to show significant difference. Therefore, the data sets are separated.

For freshwater, the selected acute toxicity data include crustaceans, fish, amphibians, and protozoans. A toxicity study with algae is also available in which the EC50 was higher than 1000 mg/L, and consequently the base-set can be considered complete. In a chronic study with algae, the NOEC for growth was 875 mg/L. Other chronic toxicity studies include bacteria, blue-green algae (cyanophyta), and protozoans. Due to the lack of chronic toxicity data for other trophic levels, the MPC has to be based on the acute toxicity data. Although especially protozoans seem to be a sensitive species for 1-butanol, the TGD does not allow to use chronic toxicity for bacteria and protozoans to base the PNEC upon.

The MPC for freshwater is derived by dividing the lowest EC50 for freshwater species by an assessment factor of 1000. The resulting MPC for freshwater is 0.22 mg/L. For saltwater species, the MPC is based on the lowest EC50 for a saltwater species divided by an assessment factor of 10000. The resulting MPC for saltwater is 0.21 mg/L.

The SRC_{eco} is derived by comparing the geometric mean of the acute toxicity data divided by an assessment factor of 10 with the geometric mean of the chronic toxicity data. Chronic toxicity data are only available for freshwater species. The geometric mean of chronic toxicity data is 94 mg/L. This is more than ten times lower than the geometric mean of the acute toxicity data for both freshwater and saltwater species. Therefore, the SRC_{eco} for both freshwater and saltwater is 94 mg/L. This value is comparable to 76 mg/L, the value found by Crommentuijn *et al.* (1995) on the basis of the combined data for the two congeners.

Table 18. Selected toxicity data for 1-butanol; freshwater and marine species.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Daphnia magna	Crustacea	1905[a]
Carassius auratus	Pisces	1900
Lepomis macrochirus	Pisces	224 [b]
Leuciscus idus melanotus	Pisces	1428 [c]
Pimephales promelas	Pisces	1858 [d]
Semotilus atromaculatus	Pisces	1183 [e]
Xenopus laevis	Amphibia	1200
Spirostomum ambiguum	Protozoa	875 [f]
Tetrahymena pyriformis	Protozoa	2466
Marine acute		**L(E)C50**
Artemia salina	Crustacea	2950
Nitroca spinipes	Crustacea	2100
Alburnus alburnus	Pisces	2300
Vibrio fischeri	Bacteria	3097[g]
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	875
Pseudomonas putida	Bacteria	650
Microcystis aeruginosa	Cyanophyta	100
Chilomonas paramecium	Protozoa	28
Entosiphon sulcatum	Protozoa	55
Uronema parduczi	Protozoa	8.0

Notes

[a] geometric mean of 1855, 1880 and 1983 mg/L. Value of 16232 mg/L was not selected, because of the strong deviation from all other values. This value is suspected to be a typing error.

[b] geometric mean of the range between no and complete mortality (100-500 mg/L).

[c] geometric mean of 1200 and 1770 mg/L.

[d] geometric mean of 1730, 1910 and 1940 mg/L.

[e] geometric mean of the range between no and complete mortality (1000-1400 mg/L).

[f] most sensitive parameter (malformations).

[g] geometric mean of 3388, 2800, 3300 and 2938 mg/L. Value of 44000 mg/L was not selected, because of the strong deviation from all other values. This value is suspected to be a typing error.

4.1.2 2-Butanol

Aquatic toxicity data for 2-butanol are given in Table A1.3. For 2-butanol, less data are available for less species than for 1-butanol, and only for freshwater species. The selected toxicity data are presented in Table 19. Acute toxicity data are available for algae, crustaceans, fish, and amphibians. Chronic toxicity data are available for algae, bacteria, cyanophyta, and protozoans.

Because the chronic toxicity data comprise only unicellular taxa (algae, bacteria, cyanophyta, and protozoans), but no taxa from higher trophic levels such as crustaceans and fish, the MPCs is in first instance conservatively based on the acute toxicity data.

The lowest EC50 is 1530 mg/L for the amphibian *Xenopus leavis*. However, it appears that the lowest NOEC for algae of 95 mg/L is more than a factor of 10 lower than this value. According to the TGD the PNEC derived from the acute toxicity data should not be higher than the PNEC derived from the chronic toxicity data. Therefore, the MPC is still based on the lowest NOEC divided by an assessment factor of 100. The resulting MPC for freshwater is 0.95 mg/L. For saltwater an assessment factor of 1000 is applied and the resulting MPC is 0.095 mg/L.

For 2-butanol, the geometric means of acute and chronic toxicity data are 3141 and 521 mg/L, respectively. The SRC_{eco} is derived from the acute toxicity data with an assessment factor of 10. The resulting SRC_{eco} is 310 mg/L.

Table 19. Selected toxicity data for 2-butanol; freshwater species.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Chlorococcales	Algae	3400
Daphnia magna	Crustacea	3316 [a]
Carassius auratus	Pisces	4300
Leuciscus idus melanotus	Pisces	3530 [b]
Pimephales promelas	Pisces	3670
Xenopus laevis	Amphibia	1530
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	95
Pseudomonas putida	Bacteria	500
Microcystis aeruginosa	Cyanophyta	312
Chilomonas paramecium	Protozoa	745
Entosiphon sulcatum	Protozoa	1282
Uronema parduczi	Protozoa	1416

Notes

[a] geometric mean of 3750, 2300 and 4227 mg/L.

[b] geometric mean of 3520 and 3540 mg/L.

4.1.3 *n*-Butyl acetate

Selected aquatic toxicity data for *n*-butyl acetate are given in Table 20. The full data set is shown in Table A1.4. Acute toxicity data are available for algae, crustaceans and fish in the case of freshwater species and for bacteria, crustaceans and fish for marine species. Chronic toxicity values are available for freshwater algae, bacteria, cyanophyta, and protozoans. As the marine toxicity data are not significantly different from the freshwater data, ERLs are based on the combined set.

Because chronic toxicity data are available for algae and additionally for three unicellular taxa, but not for crustaceans and fish, the MPCs have to be based on acute toxicity data.

The lowest EC50 is 18 mg/L for the fathead minnow (*Pimephales promelas*). With an assessment factor of 1000 the MPC for freshwater is 0.018 mg/L. For saltwater, the assessment factor is 10000 and the resulting MPC is 0.0018 mg/L.

The geometric mean of the combined set of acute toxicity data is 94 mg/L. The geometric mean of the chronic toxicity data is higher than this value. The SRC_{eco} is therefore derived from the acute toxicity data with an assessment factor of 10. The resulting SRC_{eco} is 9.4 mg/L.

The HC50 found by Posthumus *et al.* (1998) which was calculated on the basis of QSAR estimates was 89 mg/L. The HC50 found by Crommentuijn *et al.* (1995), based on experimental data, was 43 mg/L.

Table 20. Selected toxicity data for n-butyl acetate; freshwater and marine species.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Chlorococcales	Algae	1200
Daphnia magna	Crustacea	100 [a]
Lepomis macrochirus	Pisces	100
Leuciscus idus melanotus	Pisces	100 [b]
Pimephales promelas	Pisces	18
Marine acute		**L(E)C50**
Artemia salina	Crustacea	32
Menidia beryllina		185
Vibrio fischeri		70
Freshwater chronic		**NOEC**
Chlorococcales	Algae	600
Scenedesmus quadricauda	Algae	21
Pseudomonas putida	Bacteria	115
Microcystis aeruginosa	Cyanophyta	280
Chilomonas paramaecium	Protozoa	670
Entosiphon sulcatum	Protozoa	321
Uronema parduczi	Protozoa	574

Notes

[a] geometric mean of 24, 205 and 205 mg/L.

[b] geometric mean of 141 and 71 mg/L.

4.1.4 Cyclohexylamine

Selected aquatic toxicity data on cyclohexylamine are given in Table 21. The full data set is available in Table A1.5. Cyclohexylamine is a basic compound with a pKa value of 10.68. This means that under neutral pH the compound is protonated. When this compound is added to a test system it may significantly increase the pH. For all of the toxicity studies reported in Table A1.5 it was studied, whether such a pH effect could be excluded. Only in these cases toxicity data were considered valid. Data with a possible pH effect were not selected, because a pH value of above 10 is not relevant for the field situation. These data are tabulated as rejected data (Table A1.6). Differences in toxicity due to a pH effect of cyclohexylamine are most evident for *Pseudomonas putida*.

Acute toxicity data are available for algae, crustaceans, fish and protozoans. Chronic toxicity values are available for algae, bacteria, cyanophyta, and protozoans. No data for marine species are available. The most sensitive species for cyclohexylamine is the blue-green alga *Microcystis aeruginosa*, with a NOEC value of 0.02 mg/L, which is far lower than the lowest acute toxicity data. Also the available NOECs for the green alga *Scenedesmus quadricauda* are a factor of 100 lower than the lowest acute values. In that case, an assessment factor of 100 is applied to the lowest NOEC to obtain the MPC for freshwater. The resulting MPC is 0.2 µg/L. For the MPC for marine water an assessment factor of 1000 is applied to the lowest NOEC. This leads to an MPC of 0.02 µg/L.

The geometric mean of the acute and chronic toxicity data are 73 and 1.2 mg/L, respectively. The SRC_{eco} is equivalent to the geometric mean of NOEC values, i.e. 1.2 mg/L.

Table 21. Selected toxicity data for cyclohexylamine; freshwater species.

Species	**Taxon**	**Value [mg/L]**
Freshwater acute		**L(E)C50**
Chlorococcales	Algae	49
Daphnia magna	Crustacea	61 [a]
Leuciscus idus melanotus	Pisces	106 [b]
Oncorhynchus mykiss	Pisces	90
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	0.40 [c]
Pseudomonas putida	Bacteria	420
Microcystis aeruginosa	Cyanophyta	0.02
Entosiphon sulcatum	Protozoa	0.69

Notes

[a] geometric mean of 49, 80, and 58 mg/L, the test system belonging to the lowest value is buffered sufficiently. For the other two studies with this is unknown, but the possible change in pH does obviously not result in an additional toxic effect.

[b] geometric mean of 58 and 195 mg/L.

[c] geometric mean of 0.32 and 0.51 mg/L.

4.1.5 Diethylene glycol

Selected aquatic toxicity data for diethylene glycol are given in Table 22 below. The full data set is shown in Table A1.7. Rejected data are presented in Table A1.8. The acute toxicity data differ by at most a factor of 5, while the lowest chronic value is less than a factor of 50 lower than the highest acute value.

Acute toxicity data for freshwater species are available for crustaceans, fish, amphibians, and protozoans. Acute marine toxicity values are found for algae, crustaceans, fish, and bacteria. The acute toxicity data for freshwater and saltwater are not significantly different and consequently, both sets are combined. As a result the base-set (algae, *Daphnia*, fish) is complete. Chronic toxicity values are available for algae, bacteria, cyanophyta, and protozoans.

With a complete base-set, an assessment factor of 1000 is applied to the lowest EC50. The lowest EC50 is 15000 mg/L for the malformations of the African clawed frog (*Xenopus laevis*). The lowest chronic toxicity value of 1700 mg/L for the blue-green alga *Microcystis aeruginosa* is lower than this value but within a factor of 10. Therefore, the MPC is 15 mg/L. For the marine environment an assessment factor of 10000 is applied. The resulting MPC for saltwater is 1.5 mg/L.

The geometric mean of the acute and chronic toxicity data are 40831 and 4457 mg/L, respectively. The SRC_{eco} is derived from the geometric mean of the acute toxicity data with an assessment factor of 10. The resulting SRC_{eco} is 4100 mg/L. This value is comparable to the HC50 of 3598 mg/L found by Crommentuijn *et al.* (1995).

Table 22. Selected toxicity data for diethylene glycol; freshwater and marine species.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Daphnia magna	Crustacea	47200
Oncorhynchus mykiss	Pisces	57645 [a]
Pimephales promelas	Pisces	75200
Poecilia reticulata	Pisces	61000
Xenopus laevis	Amphibia	14719 [b]
Tetrahymena pyriformis	Protozoa	25860 [c]
Marine acute		**L(E)C50**
Skeletonema costatum	Algae	40800
Mysidopsis bahia	Crustacea	36900
Cyprinodon variegatus	Pisces	62100
Vibrio fischeri	Bacteria	29000
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	2700
Pseudomonas putida	Bacteria	8000
Microcystis aeruginosa	Cyanophyta	1700
Entosiphon sulcatum	Protozoa	10745

Notes

[a] geometric mean of 52800 and 62934 mg/L.

[b] geometric mean of 18740, 17470, and 9740 mg/L for the most sensitive endpoint (malformations).

[c] geometric mean of 22500, 24400, and 31500 mg/L.

4.1.6 Ethyl acetate

Selected aquatic toxicity data for ethyl acetate are given in Table 23 below. The full data set is shown in Table A1.9. Rejected data are tabulated in Table A1.10, Acute toxicity data are available for as much as 11 taxonomic groups (see also Figure 2). Most data are for freshwater species with algae, crustaceans, fish, amphibians, annelids, coelenterates, insects, molluscs, flatworms, and protozoans. Marine toxicity data are available for crustaceans and bacteria. The acute toxicity data range by a factor of 50. The lowest chronic values are up to 20 times as low as the lowest acute value.

The lowest acute value is 110 for the protozoan *Tetrahymena thermophila*. Chronic toxicity are available for algae, daphnids, bacteria, blue-green algae, and protozoans. The lowest values are for *Daphnia magna* and the protozoan *Tetrahymena thermophila*, based on nominal concentrations. The results based on measured concentrations for *Daphnia magna* is the lowest value and used to derive the MPC. With an assessment factor of 50, the MPC is 0.11 mg/L. For the marine environment, an assessment factor of 500 is used. Consequently, the MPC for saltwater is 0.011 mg/L.

The geometric mean of the acute toxicity data is 660 mg/L. The geometric mean of the chronic toxicity data is 243 mg/L. The SRC_{eco} is derived from the acute toxicity data with an assessment factor of 10 and is 66 mg/L. This value is lower than the value of 527 mg/L found by Posthumus *et al*. (1998) and calculated on the basis of QSARs.

Table 23. Selected toxicity data for ethyl acetate; freshwater and marine species.

Species	**Taxon**	**Value [mg/L]**
Freshwater acute		**L(E)C50**
Chlorococcales	Algae	4300
Scenedesmus subspicatus	Algae	5600 [a]
Selenastrum sp.	Algae	2500
Asellus aquaticus	Crustacea	1600
Daphnia cucullata	Crustacea	164 [b]
Daphnia magna	Crustacea	711 [c]
Daphnia pulex	Crustacea	260 [d]
Gammarus pulex	Crustacea	750
Leuciscus idus melanotus	Pisces	300 [e]
Oncorhynchus mykiss	Pisces	333 [f]
Oryzias latipes	Pisces	335 [g]
Pimephales promelas	Pisces	243 [h]
Poecilia reticulata	Pisces	210
Ambystoma mexicanum	Amphibia	150
Xenopus laevis	Amphibia	180
Tubificidae	Annelida	760
Erpobdella octoculata	Annelida	1200
Hydra ologactis	Coelenterata	1350
Aedes aegypti	Insecta	350
Chironomus thummi	Insecta	750
Cloëon dipterum	Insecta	480
Corixa punctata	Insecta	600
Culex pipiens	Insecta	3950
Ischnura elegans	Insecta	600
Nemoura cinera	Insecta	130
Lymnea stagnalis	Mollusca	1100
Dugesia lugubris	Platyhelminthes	3020
Tetrahymena thermophila	Protozoa	110 [i]
Marine acute		**L(E)C50**
Vibrio fischeri	Bacteria	5188
Artemia salina	Crustacea	708 [j]
Freshwater chronic		**NOEC**
Chlorococcales	Algae	1000
Pseudokirchneriella subcapitata	Algae	2000
Scenedesmus quadricauda	Algae	15
Daphnia magna	Crustacea	5.4 [k]
Pseudomonas putida	Bacteria	650
Microcystis aeruginosa	Cyanophyta	550
Tetrahymena thermophila	Protozoa	12
Chilomonas paramaecium	Protozoa	3248
Entosiphon sulcatum	Protozoa	202
Uronema parduczi	Protozoa	1620

Notes

[a] most relevant endpoint (growth rate).

[b] geometric mean of 175 and 154 mg/L.

[c] geometric mean of 660, 560, 819, 778, 698, and 786 mg/L for exposure time of 48 h.

[d] geometric mean of 230 and 795 mg/L.
[e] geometric mean of 270 and 333 mg/L.
[f] geometric mean of 230, 260, 484, and 425 mg/L for exposure time of 48 and 96 h.
[g] geometric mean of 125 and 900 mg/L for temperature range of 20-24 °C.
[h] longest exposure time of 96 h.
[I] geometric mean of 100 and 120 mg/L.
[j] geometric mean of 1590, 645, and 346 mg/L for mortality/immobility.
[k] geometric mean of range of measured concentrations (2.4-12 mg/L).

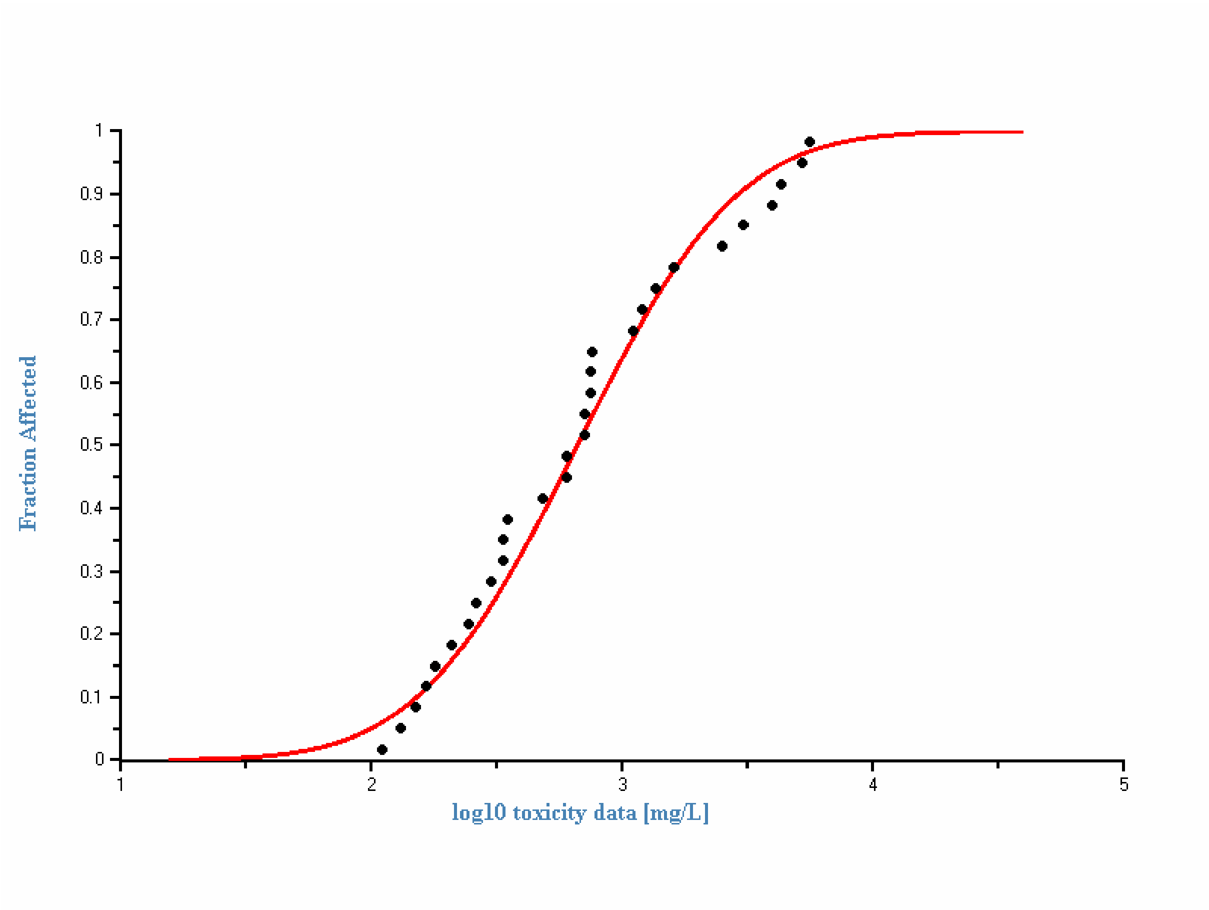


Figure 2. Distribution of acute toxicity data for ethyl acetate to species belonging to 11 taxonomic groups.

4.1.7 Ethylene glycol

Selected aquatic toxicity data for ethylene glycol are given in Table 24. The full data set of accepted and rejected data is reported in Table A1.11 and Table A1.12, respectively. Acute toxicity data for freshwater species are available for nine taxonomic groups, which are algae, crustaceans, fish, amphibians, fungi, insects, plants, protozoans and rotifers. Acute toxicity data for saltwater species include algae, crustaceans, fish, and rotifers. The acute toxicity data for freshwater and saltwater species are significantly different (P=0.02). Similar to 1-butanol, the values for saltwater species are higher than for freshwater species. This effect is also observed, if data for algae, crustaceans, fish, or rotifers are considered separately. However, each of these data sets is too small to show significant differences between freshwater and saltwater species. Chronic toxicity data are available for algae, crustaceans (daphnids), fish, bacteria, blue-green algae, insects, protozoans, rotifers. The range of acute toxicity data is a factor of 33 and for the separate sets of freshwater and saltwater data the range is within a factor of 17 and 7, respectively.

Table 24. Selected toxicity data for ethylene glycol; freshwater and marine species.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Pseudokirchneriella subcapitata	Algae	5409
Ceriodaphnia dubia	Crustacea	17921 [a]
Daphnia magna	Crustacea	49224 [b]
Daphnia pulex	Crustacea	60406
Streptocephalus proboscideus	Crustacea	54496
Procambarus sp.	Crustacea	91430
Lepomis macrochirus	Pisces	27540
Oncorhynchus mykiss	Pisces	37122 [c]
Pimephales promelas	Pisces	59304 [d]
Poecilia reticulata	Pisces	49300
Xenopus laevis	Amphibia	12978 [e]
Geotrichum	Fungae	74482
Chironomus tentans	Insecta	15596
Lemna gibba	Macrophyta	10920
Tetrahymena pyriformis	Protozoa	10515
Chilomonas paramaecium	Protozoa	53200
Colpidium campylum	Protozoa	28090
Brachionus calyciflorus	Rotifera	26461
Marine acute		**L(E)C50**
Skeletonema costatum	Algae	44200
Artemia salina	Crustacea	180618
Crangon crangon	Crustacea	50000
Mysidopsis bahia	Crustacea	34200
Cyprinodon variegatus	Pisces	27600
Sciaenops ocellatus	Pisces	145000
Brachionus plicatilis	Rotifera	149584
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	> 10000
Ceriodaphnia dubia	Crustacea	5459 [f]
Oncorhynchus mykiss	Pisces	14692
Pimephales promelas	Pisces	12531 [g]
Microcystis aeruginosa	Cyanophyta	2000
Chironomus tentans	Insecta	4567
Chilomonas paramaecium	Protozoa	112
Brachionus plicatilis	Rotifera	12800

Notes

[a] geometric mean of 29700, 22600, 25500, 13900, 10500, 6900, 34440 mg/L.

[b] geometric mean of 51000, 4110, 47400, 57600, 45500, 51000, 46300, 50450, and 54700 mg/L for all individual tests with an exposure time of 48 h.

[c] geometric mean of 45700, 17800, 41000, 56481, 60827, 22810, 24591, 41000, and 50800 mg/L for different length and weight.

[d] geometric mean of 68275, 69516, 53000, 49000, 57000, 50400, and 72860 mg/L for the standard test duration of 96 h and endpoint mortality.

[e] geometric mean of 12570, 10470, and 16610 mg/L for the lowest endpoint (malformations).

[f] geometric mean of 8590 and 3469 mg/L for the most sensitive endpoint (reproduction).

[g] most sensitive endpoint (growth).

The lowest chronic NOEC or EC10 is 112 mg/L for the protozoan *Chilomonas paramaecium*. However, according to the TGD, only acute toxicity data for bacteria and protozoans are used to base the PNEC upon. Moreover, two values from two different studies are available for this species, one for mortality and one for growth. These two values differ by a factor of 357. Therefore, the validity of the number can be questioned. The MPC is derived from the second lowest value of 2000 mg/L for the blue-green algae *Microcystis aeruginosa*. With chronic toxicity data for algae, daphnids and fish, the applied assessment factor is 10. The resulting MPC for freshwater is 200 mg/L. For saltwater the MPC is 20 mg/L, derived by application of an assessment factor of 100.

The geometric means of the acute toxicity data for freshwater and saltwater are 28675 and 68289 mg/L, respectively. The geometric mean of the chronic toxicity data is 3877 mg/L. The geometric mean for the freshwater data is less than 10 times higher and consequently, the SRC_{eco} is based on this value: 2900 mg/L. This value is more than a factor of 4 higher than the value of 676 mg/L found by Crommentuijn *et al.* (1995). For saltwater, the SRC_{eco} is 6800 mg/L. The difference with the value derived by Crommentuijn *et al.* (1995) is more than a factor of 10. However, because of the uncertainty in the lowest chronic NOEC, and its influence on the geometric mean of the chronic toxicity data, the SRC_{eco} for saltwater is also based on the geometric mean of the acute toxicity data: 6800 mg/L.

4.1.8 Methanol

Selected aquatic toxicity data for methanol are given in Table 25. The full data set is available in Table A1.13 and Table A1.14, for accepted and rejected data respectively. As marine toxicity data were not significantly different from the freshwater ones (P=0.21 and P=0.93 for the acute and chronic values, respectively), ERL values are derived from the combined data set. Acute toxicity data are available for a large diversity of species. For freshwater data are available for algae, crustaceans, fish, bacteria, blue-green algae, fungi, insects, protozoans, and rotifers. For saltwater, data for algae, crustaceans, fish, bacteria, molluscs, and rotifers are available. The total set, including 10 taxonomic groups, ranges over a broad range with differences up to nearly a factor of nearly 500. The data do not follow a log-normal distribution. Chronic data for both freshwater and saltwater are restricted to unicellular species.

The base-set is complete, because acute toxicity data are available for algae, *Daphnia*, and fish. Chronic toxicity data are restricted to algae and other unicellular organisms. The lowest acute values of 180 mg/L are for two species of marine algae. Although in the right order of magnitude, there is some uncertainty in these values, because they were read from a figure. The lowest chronic values of 19 and 56 mg/L are for the same two species of algae, but these are reported in a table in the study. The lowest NOEC is 19 mg/L for an *Eutreptiella* species, which is roughly a factor of 10 lower than the EC50 values. Therefore, the MPC is derived from the lowest chronic value with an assessment factor of 100. The resulting MPC for freshwater is 0.19 mg/L. For the marine assessment, additional marine taxa such as molluscs or echinoderms are not available. Consequently, for the marine environment, an assessment factor of 1000 is applied, leading to an MPC of 0.019 mg/L.

The geometric means of the acute and chronic toxicity data set are 12178 and 1280 mg/L, respectively. The SRC_{eco} is equal to the geometric mean of the acute data divided by an assessment factor of 10: 1200 mg/L. The current SRC_{eco} is a factor of 6 higher than the value of 250 mg/L found by Crommentuijn *et al.* (1995).

Table 25. Selected toxicity data for methanol; freshwater and marine species.

Species	**Taxon**	**Value [mg/L]**
Freshwater acute		**L(E)C50**
Chlorella pyroneidosa	Algae	28490
Chlorella vulgaris	Algae	2610
Chlorella zofingiensis	Algae	7113
Chlorococcales	Algae	12000
Daphnia magna	Crustacea	6782 [a]
Daphnia obtusa	Crustacea	22200
Daphnia pulex	Crustacea	23172 [b]
Hyalella azteca	Crustacea	19389
Streptocephalus proboscideus	Crustacea	32681
Lepomis macrochirus	Pisces	15400 [c]
Oncorhynchus mykiss	Pisces	17364 [d]
Pimephales promelas	Pisces	28743 [e]
Poecilia reticulata	Pisces	10860
Nitrosomonas sp.	Bacteria	880
Anabaena cylindrica	Cyanophyta	20339
Anabaena inaequalis	Cyanophyta	21210
Anabaena variabilis	Cyanophyta	24771
Anabaena sp.	Cyanophyta	24692
Nostoc sp.	Cyanophyta	43369
Geotrichum candidum	Fungae	48060
Culex restuans	Insecta	20022
Paramecium caudatum	Protozoa	7690
Spirostomum ambiguum	Protozoa	17590
Tetrahymena pyriformis	Protozoa	18756
Brachionus calyciflorus	Rotifera	35885
Marine acute		**L(E)C50**
Chaetoceros calcitrans	Algae	13000
Dunaliella tertiolecta	Algae	18000
Eutreptiella sp.	Algae	180
Hetersigma akashiwo	Algae	180
Isochrysis galbana	Algae	17000
Pavlova lutheri	Algae	15000
Prorocentrum minimum	Algae	2600
Skeletonema costatum	Algae	6500
Tetraselmis tetrathele	Algae	22000
Artemia salina	Crustacea	5049 [f]
Nitroca spinipes	Crustacea	12000
Palaemonetes kadiakensis	Crustacea	21922
Crangon crangon	Crustacea	1345
Alburnus alburnus	Pisces	28000
Agonus cataphractus	Pisces	14376 [g]
Sciaenops ocellatus	Pisces	88000
Vibrio fischeri	Bacteria	42108 [h]
Cerastoderma edule	Mollusca	4547 [i]
Mytilus edulis	Mollusca	15200

Brachionus placitilis	Rotifera	51905
Freshwater chronic		**NOEC**
Chlorella vulgaris	Algae	791
Chlorella zofingiensis	Algae	801
Chlorococcales	Algae	1600
Pseudokirchneriella subcapitata	Algae	791
Scenedesmus quadricauda	Algae	8000
Pseudomonas putida	Bacteria	6600
Microcystis aeruginosa	Cyanophyta	530
Chilomonas paramaecium	Protozoa	441
Marine chronic		**NOEC**
Chaetoceros calcitrans	Algae	4432
Dunaniella tertiolecta	Algae	7914
Eutreptiella sp.	Algae	19
Heterosigma akashiwo	Algae	56
Isochrysis galbana	Algae	6410
Pavlova lutheri	Algae	4511
Prorocentrum minimum	Algae	324
Skeletonema costatum	Algae	1108
Tetraselmis tetrathele	Algae	11080
Vibrio fischeri	Bacteria	1995[j]

[a] geometric mean of 24500, 1983, 13240, 3289 mg/L for the exposure time of 48 h.
[b] geometric mean of 19548 and 27468 mg/L.
[c] longest exposure time (96 h).
[d] geometric mean of 15000 and 20100 mg/L.
[e] geometric mean of 29400 and 28100 mg/L.
[f] geometric mean of 1579, 1101, 901, 43574, and 48060 mg/L for mortality.
[g] geometric mean of 7914 and 26116 mg/L.
[h] geometric mean of 42000, 125000, 14736, 29348 and 58303 mg/L.
[i] geometric mean of 2612 and 7914 mg/L.
[j] NOEC = LOEC (less than 20% effect) divided by 2.

4.1.9 Methyl ethyl ketone

Selected aquatic toxicity data for methyl ethyl ketone (MEK) are given in Table 26. All underlying data are shown in Table A1.15 and Table A1.16, for accepted and rejected toxicity data, respectively. The acute toxicity data for the two marine species are not significantly different from the rest. Therefore, these sets are combined. Chronic toxicity data are only available for freshwater species for unicellular species.

There is only one study for acute toxicity to algae, which did not results in a valid EC50. The highest concentration tested is still lower than the lowest valid EC50 of the rest of the species. Therefore, the base-set is in principle not complete. However, there is a chronic NOEC for algae, which compensates this missing acute value for algae. The value of this NOEC for *Scenedesmus quadricauda* is 4300 mg/L, which is well above the lowest LC50s of 2400 mg/L for the goldfish and 1950 mg/L for the marine crustacean *Artemia salina*. The lowest NOEC for the blue-green algae *Microcystis aeruginosa* of 120 mg/L is substantially lower than these values. Therefore, the MPC for freshwater is derived from this value with an assessment factor of 100: 1.2 mg/L. For the marine environment a higher assessment factor of 1000 is applied, resulting in an MPC of 0.12 mg/L.

The geometric means of the acute and chronic toxicity data are 4076 and 992 mg/L, respectively. The **SRC$_{eco}$** based on the acute data is **410 mg/L**. This value is lower than the value of 973 mg/L found by Crommentuijn *et al*. (1995).

Table 26. Selected toxicity data for methyl ethyl ketone; freshwater and marine organisms.

Species	**Taxon**	**Value [mg/L]**
Freshwater acute		**L(E)C50**
Daphnia magna	Crustacea	5091 [a]
Carassius auratus	Pisces	2400
Lepomis macrochirus	Pisces	5640
Leuciscus idus melanotus	Pisces	4738 [b]
Pimephales promelas	Pisces	3220
Poecilia reticulata	Pisces	5700
Tetrahymena pyroformis	Protozoa	6000
Marine acute		**L(E)C50**
Artemia salina	Crustacea	1950
Vibrio fischeri	Bacteria	4430 [c]
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	4300
Pseudomonas putida	Bacteria	1150
Microcystis aeruginosa	Cyanophyta	120
Chilomonas paramaecium	Protozoa	2982
Entosiphon sulcatum	Protozoa	190
Uronema parduczi	Protozoa	2830

Notes
[a] longest exposure time (48 h).
[b] geometric mean of 4600 and 4880 mg/L.
[c] geometric mean of 3886 and 5050 mg/L.

4.1.10 Tribromomethane

Aquatic toxicity data on tribromomethane (bromoform) are given in Table A1.17. Selected data are shown in Table 27. The sensitivity of fresh water and marine species differed significantly (P=0.02). If algae, crustaceans and fish are regarded separately, the values for marine species are lower in each case. Consequently, if the set of one species of algae and two species of both crustaceans and fish is considered, the difference between freshwater and the saltwater species is still highly significant (P=0.004). Chronic values are only available for freshwater algae and saltwater fish. Because of this limited number of studies, the chronic data can not be tested for differences between freshwater and saltwater species.

For freshwater, the base-set is complete. The lowest LC50 is 29 mg/L for the fish *Lepomis macrochirus*. Only one chronic NOEC of 10 mg/L is available for an algae species. Applying an assessment factor of 1000 to the lowest acute value, would lead to a value of 0.029 mg/L. However, by doing so, the data for marine species, which are more sensitive in acute tests, are completely disregarded. If the chronic data for marine species are considered as well, chronic data for both algae and fish are available. Because the most sensitive species for freshwater species is the fish, an assessment factor of 50 has to be applied to the lowest NOEC, which is 4.8 mg/L for *Cyprinodon variegatus*. This leads to an MPC for freshwater of 0.096 mg/L. Considering the fact that the difference in interspecies sensitivity for acute effects is less than a factor of 2 and the acute-to-chronic ratio for the algae *Pseudokirchneriella subcapitata* is only 4, this MPC is protective for the aquatic environment.

For saltwater, data are available for algae, crustaceans, and fish as well. However, the lowest acute value is the LC50 of 1.5 mg/L for the mollusc *Crassostrea virginica*. With one chronic NOEC for fish and one additional NOEC for a freshwater algae but not for the most sensitive taxonomic group of acute toxicity to saltwater species (molluscs), the assessment factor to be applied should be 1000. However, the lowest L(E)C50 is lower than the lowest NOEC. According to the TGD, this factor should therefore be applied to the lowest L(E)C50. The resulting MPC for saltwater is 0.0015 mg/L. The presented dose-response relationship for *Crassostrea virginica* (Stewart *et al.*, 1979), does not allow to establish an exact value for the EC10, but an estimate of the EC10 is around 0.05 mg/L. Thus, applying an assessment factor of 1000 to the EC50 should be considered as protective for this species.

The geometric mean of the acute toxicity data for freshwater species is 41 mg/L. The geometric of the two chronic data is 6.9 mg/L. Consequently, the SRC_{eco} for freshwater is 4.1 mg/L. This result is almost a factor of 10 lower than the value of 34 mg/L found by Posthumus *et al.* (1998) who calculated an HC50 for aquatic species on the basis of QSARs. The geometric mean of the acute toxicity data for saltwater species is 10 mg/L. Therefore, the SRC_{eco} for saltwater is 1.0 mg/L.

Table 27. Selected toxicity data for tribromomethane; freshwater and marine organisms.

Species	Taxon	Value [mg/L]
Freshwater acute		**L(E)C50**
Pseudokirchneriella subcapitata	Algae	40.1[a]
Daphnia magna	Crustacea	46
Daphnia pulex	Crustacea	44
Cyprinus carpio	Pisces	52 [b]
Lepomis macrochirus	Pisces	29
Marine acute		**L(E)C50**
Skeletonema costatum	Algae	12.3
Americamysis bahia	Crustacea	24.4
Penaeus aztecus	Crustacea	26
Cyprinodon variegatus	Pisces	7.1 [c]
Brevoortia tyrannus	Pisces	12
Crassostrea virginica	Mollusca	1.5
Freshwater chronic		**NOEC**
Pseudokirchneriella subcapitata	Algae	10
Marine chronic		**NOEC**
Cyprinodon variegatus	Pisces	4.8

Notes

[a] Most relevant parameter (growth rate) for *Pseudokirchneriella subcapitata*.

[b] LC50 based on actual concentrations.

[b] Most reliable LC50 value for *Cyprinodon variegatus* based on actual concentrations.

4.1.11 Triethanolamine

Selected aquatic toxicity data for triethanolamine are given in Table 28. The complete data set is given in Table A1.18 and Table A1.19, for accepted and rejected toxicity data respectively. Similar to cyclohexylamine, triethanolamine is a basic compound. Its pKa value (7.76) is lower than that of cyclohexylamine. When this compound is added to a test system it may significantly increase the pH, but at higher concentrations than for cyclohexylamine. For all of the toxicity studies reported in Table A1.18 it was studied, whether such a pH effect could be excluded. Only in these cases toxicity data were considered valid. Data with a possible pH effect were not selected, because such data are not relevant for the field situation. These data are tabulated as rejected data (Table A1.19). Large differences in toxicity were found for *Scenedesmus quadricauda* between neutralized and not neutralized solutions. Contrary to what is expected, the compound was more toxic at pH 7 than when the solutions were not neutralized. Therefore, the geometric mean of both NOECs is the selected value for this species. This value is also more in line with the value for the other closely related algae species *Scenedesmus subspicatus*.

Acute toxicity data for freshwater species comprise algae, daphnids (*Daphnia*) and fish. No accepted toxicity data are available for saltwater species. Chronic toxicity data are only available for freshwater species and include algae, *Daphnia*, bacteria, blue-green algae, and protozoans.

The base-set for triethanolamine is complete. The most sensitive species among the acute toxicity data is the algae *Scenedesmus subspicatus*. The toxicity study with the daphnid *Ceriodaphnia dubia*, for which the pH is unknown, showed almost equal sensitivity of this species, provided that this effect is not caused by a change in pH.

There are chronic toxicity data for algae and daphnids (*Daphnia*). Therefore, an assessment factor of 50 can be applied to the lowest NOEC. This is the NOEC of 16 mg/L for the daphnid *Daphnia magna*. The resulting MPC for freshwater is 0.32 mg/L. For saltwater, with an assessment factor of 500, the MPC is 0.032 mg/L.

The geometric mean of the acute and chronic toxicity data are 3046 and 82 mg/L, respectively. The SRC_{eco} is based on the chronic data set and is 82 mg/L.

Table 28. Selected toxicity data for triethanolamine; freshwater and marine organisms.

Species	**Taxon**	**Value [mg/L]**
Freshwater acute		**L(E)C50**
Scenedesmus subspicatus	Algae	750 [a]
Daphnia magna	Crustacea	1737 [b]
Pimephales promelas	Pisces	11800
Freshwater chronic		**NOEC**
Scenedesmus quadricauda	Algae	36 [c]
Scenedesmus subspicatus	Algae	110 [a]
Daphnia magna	Crustacea	16
Microcystis aeruginosa	Cyanophyta	47
Chilomonas paramecium	Protozoa	1768
Entosiphon sulcatum	Protozoa	56

Notes

[a] Most relevant parameter (growth rate).

[b] Geometric mean of 1390, 1850, and 2038 mg/L.

[c] Geometric mean of 750 and 1.8 mg/L.

4.1.12 Summary of derived ERLs for the aquatic compartment

In Table 29 an overview of the derived ERLs for the aquatic compartment are given. The negligible concentrations are derived from the MPC values by dividing the MPC by a factor of 100.

Table 29. Overview of derived NC, MPC and SRC_{eco} values for freshwater and marine water. Values for the total and dissolved fraction are equal.

Compound	NC fresh [mg/L]	MPC fresh [mg/L]	SRC_{eco} fresh [mg/L]	NC marine [mg/L]	MPC marine [mg/L]	SRC_{eco} marine [mg/L]
1-butanol	0.0022	0.22	94	0.0021	0.21	94
2-butanol	0.0095	0.95	310	$9.5 \cdot 10^{-4}$	0.095	310
n-butyl acetate	$1.8 \cdot 10^{-4}$	0.018	9.4	$1.8 \cdot 10^{-5}$	0.0018	9.4
cyclohexylamine	$2.0 \cdot 10^{-6}$	$2.0 \cdot 10^{-4}$	1.2	$2.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-5}$	1.2
diethylene glycol	0.15	15	4100	0.015	1.5	4100
ethyl acetate	0.0011	0.11	66	$1.1 \cdot 10^{-4}$	0.011	66
ethylene glycol	2.0	200	2900	0.20	20	6800
methanol	0.0019	0.19	1200	$1.9 \cdot 10^{-4}$	0.019	1200
methyl ethyl ketone	0.012	1.2	410	0.0012	0.12	410
tribromomethane	$9.6 \cdot 10^{-4}$	0.096	4.1	$1.5 \cdot 10^{-5}$	0.0015	1.0
triethanolamine	0.0032	0.32	82	$3.2 \cdot 10^{-4}$	0.032	82

4.2 Derivation of ERLs for soil and sediment

Only one study with a terrestrial plant was found for *n*-butyl acetate (Table A2.1), which is substantially higher than the value derived by equilibrium partitioning. In Posthumus *et al.* (1998), selected data for toxicity of tribromomethane to three terrestrial plants are presented, but the origin of these data is unknown. Therefore, they are not included in the current risk assessment. For the rest of the compounds, experimental data on toxicity to soil or sediment inhabiting organisms are not available. For that reason, equilibrium partitioning (EqP) is used to derive all risk limits for soil or sediment. The methods used are described in section 3.2.4 and follow the guidelines of the TGD (European Commission, 2003). Following this EU-guidance, the ERLs for sediment is set equal to the ERL for suspended matter, which is calculated from the ERLs for water using EqP. The selected values from section 2.1 are used (marked bold) for the log K_{oc}, that is used in the calculation of both sediment and soil concentrations, and the Henry's Law Constant, used in the calculation of the soil concentrations.

Bulk concentration based on wet weight are normalised to dry weight of Dutch standard soil and sediment, containing 10% organic matter. For the non-hydrophobic chemicals, described in this report, the fraction associated with solids may be very small, even less than 10% in the case of sediment. Therefore, the ERLs for sediment and soil should be used carefully, especially if the water content of the sediment or soil sample deviates substantially from the values of 90% and 20%, for suspended matter and soil respectively. The influence of the pore water content on the concentration in soil is restricted mainly to butanol, methanol, ethylene glycol, diethylene glycol, and triethanolamine, which are for more than 50% in the pore water at soil moisture content of 20%. For the other compounds less than 25% of the total amount in bulk soil is dissolved in pore water at soil moisture content of 20%. In bulk sediment, only tribromomethane, *n*-butylacetate, and cyclohexylamine are more than half associated with solid particles, with a water content of 90%.

The derived values for soil and sediment are presented in Table 30 and Table 31.

For soil, Crommentuijn *et al.* (1995) derived the values of 76 mg/kg for butanol, 95 mg/kg for butyl acetate, 450000 mg/kg for diethylene glycol, 90 mg/kg for ethylene glycol, 33 mg/kg for methanol, and 175 mg/kg for methyl ethyl ketone. Posthumus *et al.* (1998) derived the values of 196 mg/kg for butyl acetate, 68 mg/kg for ethyl acetate, and 300 mg/kg for tribromomethane, on basis of QSARs. Changes in SRC_{eco} values are mostly caused by the derivation of different SRC$_{eco}$ values for water, on which they are based. Other aspects that influence the derived values, are the used K_{oc} values and the recalculation from wet weight to dry weight.

Table 30. Overview of derived NC, MPC and SRC$_{eco}$ values for soil. Values are normalised to dry weight.

Compound	NC [mg/kg$_{dw}$]	MPC [mg/kg$_{dw}$]	SRC$_{eco}$ [mg/kg$_{dw}$]
1-butanol	0.0015	0.15	63
2-butanol	0.0068	0.68	220
n-butyl acetate	$9.6 \cdot 10^{-4}$	0.096	50
cyclohexylamine	$8.1 \cdot 10^{-6}$	$8.1 \cdot 10^{-4}$	5.0
diethylene glycol	0.066	6.6	1800
ethyl acetate	0.0020	0.20	130
ethylene glycol	0.89	89	1300
methanol	$9.8 \cdot 10^{-4}$	0.098	630
methyl ethyl ketone	0.022	2.2	750
tribromomethane	0.011	1.1	46
triethanolamine	0.0019	0.19	47

Table 31. Overview of derived NC, MPC and SRC$_{eco}$ values for freshwater and sediment. Values are normalised to dry weight.

Compound	NC fresh [mg/kg$_{dw}$]	MPC fresh [mg/kg$_{dw}$]	SRC$_{eco}$ fresh [mg/kg$_{dw}$]	NC marine [mg/kg$_{dw}$]	MPC marine [mg/kg$_{dw}$]	SRC$_{eco}$ marine [mg/kg$_{dw}$]
1-butanol	0.0054	0.54	230	0.0050	0.50	230
2-butanol	0.023	2.3	770	0.0023	0.23	770
n-butyl acetate	0.0013	0.13	66	$1.3 \cdot 10^{-4}$	0.013	66
cyclohexylamine	$1.2 \cdot 10^{-5}$	0.0012	7.2	$1.2 \cdot 10^{-6}$	$1.2 \cdot 10^{-4}$	7.2
diethylene glycol	0.32	32	8900	0.032	3.2	8900
ethyl acetate	0.0039	0.39	240	$3.9 \cdot 10^{-4}$	0.039	240
ethylene glycol	4.3	430	6200	0.43	43	15000
methanol	0.0043	0.43	2700	$4.3 \cdot 10^{-4}$	0.043	2700
methyl ethyl ketone	0.043	4.3	1500	0.0043	0.43	1500
tribromomethane	0.012	1.2	53	$1.9 \cdot 10^{-4}$	0.019	13
triethanolamine	0.0074	0.74	190	$7.4 \cdot 10^{-4}$	0.074	190

5. Conclusions

In this report maximum permissible concentrations (MPCs), negligible concentrations (NCs) and Serious Risk Concentrations for (SRC_{eco}s) for water, soil and sediment were derived for an heterogeneous group of eleven compounds. Nine out of the eleven compounds have already been evaluated by Crommentuijn *et al.* (1995) and Posthumus *et al.* (1998), who derived SRCs for soil.

For the compounds 1-butanol and diethylene glycol the differences in SRC_{eco} for water reported in this report and the ones found by Crommentuijn *et al.* (1995) were small, i.e. less than 25%, both values derived here being slightly higher. For 2-butanol, which was not distinguished from 1-butanol in the value from Crommentuijn *et al.* (1995), and for ethylene glycol and methanol, the values derived here are a factor of 4 to 5 higher than the old values. For *n*-butyl acetate, ethyl acetate, ethylene glycol, methyl ethyl ketone, and tribromomethane, the new values are a factor of 2 to 10 higher. This is probably due to three reasons: (1) the use of QSARs instead of experimental data in the derivation of some of the old SRC values, (2) the larger amount of experimental data available since 1995, and (3) differences in the method used for the derivation of HC50.

For the terrestrial and sediment compartments, experimental toxicity data were limited to only one study for one compound. Consequently, ERLs for these compartments were derived on the basis of the equilibrium partitioning method. Experimental sorption coefficients (K_{oc}) were available for 1-butanol, methanol, methyl ethyl ketone, and tribromomethane. For the rest of the compounds, no experimental values could be found. The used log K_{oc} values were an average value of the experimental values, if available, and log K_{oc} values, calculated using the empirical regression equations of Sabljić *et al.* (1995), using the log K_{ow}.

For most of the compounds considered in this report (with the exception of diethylene glycol), the differences in SRC_{eco} values for soil between the studies of Posthumus *et al.* (1998) and Crommentuijn *et al.* (1995), and the current study, range from a factor of 2 to 20. The discrepancies between the current evaluation and the studies of Posthumus *et al.* (1998) and Crommentuijn *et al.* (1995) are mainly caused by (1) differences in HC50 for aquatic species due to the larger amount of toxicity data, (2) differences in the method used for the derivation of HC50, (3) the differences in sorption coefficients (K_{oc}), and (4) the normalisation of bulk concentrations in soil (wet weight) to dry weight according to the TGD. Because of the normalisation of wet to dry weight, most SRC_{eco} values are higher than the values derived before.

The use of the equilibrium partitioning method and the use of regression models to estimate the partition coefficient (K_p) for soil or sediment brings some uncertainty with it. However, the estimated log K_{oc} values are based on well-established relationships with reliable values for log K_{ow} as input. When available, experimental values for log K_{oc} were close to estimated values (difference 0.2-0.3 log-unit). However, availability of experimental toxicity data for soil or sediment would increase the reliability of the risk limits for these compartments.

The derivation of MPCs based on the TGD guidance, using assessment factors for most substances, leads to more stringent risk limits when compared to the previous INS method (Traas, 2001). In general, application of TGD guidance leads to MPCs that are at least a factor of 10 more strict than when statistical extrapolation would have been used (former INS methodology).

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Appendix 1. Information on aquatic toxicity

Legend

Species	species used in the test, if available followed by age, size, weight or life stage
Analysed	Y = test substance analysed in test solution N = test substance not analysed in test solution or no data
Test type	S = static, Sc = static with closed test vessels, R = static with renewal, F = flow through
Substance purity	percentage active ingredient, or chemical grade of purity.
Hardness/salinity	freshwater: hardness expressed as mg $CaCO_3$/L saltwater: salinity expressed in ‰
Test water	am = artificial medium, dtw = dechlorinated tap water, dw = dechlorinated water, nw = natural water, rw = reconstituted water (+additional salts), tw = tap water
Exposure time	h = hours, d = days, w = weeks, m = months, min. = minutes
Criterion	L(E)Cx = test result showing x% mortality (LCx) of effect (ECx). LC50s and EC50s are usually determined for acute effects, EC10s are for chronic effects; NOEC = no observed effect concentration, statistically determined

Contents

Table A1.1. Accepted toxicity data for 1-butanol.

Species	Analysed	Test type	Substance purity	pH	Hardness Salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	>1000		Krebs (1991)
Crustacea												
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	1855		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	1880		Bringmann & Kühn (1982)
Daphnia magna, 6-24 h	N	Sc	-	8.0±0.2	240	am	48 h	EC50	immobility	1983		Kühn *et al*. (1989a)
Pisces												
Carassius auratus, 6.2±0.7 cm, 3.3±1.0 g	Y	S	-	7.8	283	tw	24 h	LC50	mortality	1900		Bridié *et al*. (1979)
Lepomis macrochirus, 0.1 g	N	S	tech.	7.4	270	-	96 h	LC50	mortality	100-500		Mayer & Ellersieck (1986)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	1200		Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	1770		Juhnke & Lüdemann (1978)
Oryzias latipes, 2 cm, 0.2 g	N	S	-	7.2	40	-	48 h	LC50	mortality	>1000	1	Tsuji *et al*. (1986)
Oryzias latipes, 2 cm, 0.2 g	N	S	-	7.2	40	-	48 h	LC50	mortality	500	2	Tsuji *et al*. (1986)
Pimephales promelas, 33 d, 20.6 mm, 0.119 g	Y	F	99%	7.6; 7.5	48; 45.5	nw	96 h	LC50	mortality	1730		Brooke *et al*. (1984); Veith *et al*. (1983)
Pimephales promelas, juvenile, 4-8 w, 1.1-3.1 cm	N	R	-	-	-	-	96 h	LC50	mortality	1910		Mattson *et al*. (1976)
Pimephales promelas, juvenile, 4-8 w, 1.1-3.1 cm	N	R	-	-	-	-	96 h	LC50	mortality	1940		Mattson *et al*. (1976)
Semotilus atromaculatus	N	S	-	8.3	98	-	24 h	LC50	mortality	1000-1400		Gillette *et al*. (1952)
Amphibia												
Xenopus laevis, 3-4 w	N	S	Ag	8.0	200	DSW	48 h	LC50	mortality	1200		De Zwart & Slooff (1987)
Protozoa												
Spirostomum ambiguum	N	Sc	analyt.	7.4±0.2	2.8	am	48 h	EC50	malformation/ deformation	875		Nałęcz-Jawecki & Sawicki (1999)
Spirostomum ambiguum	N	Sc	analyt.	7.4±0.2	2.8	am	48 h	LC50	mortality	1097		Nałęcz-Jawecki & Sawicki (1999)
Tetrahymena pyriformis, late log-phase	N	S	≥ 95%	-	-	-	48 h	EC50	growth	2466		Schultz *et al*. (1990); Schultz & Tichy (1993)
ACUTE TOXICITY- saltwater												
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	2950		Price *et al*. (1974)
Nitroca spinipes, adult	N	S	p.a.	7.9	7	nw	96 h	LC50	mortality	2100		Bengtsson *et al*. (1984)
Nitroca spinipes, adult	N	S	p.a.	7.8	7	nw	96 h	LC50	mortality	2100		Lindén *et al*. (1979)
Pisces												
Alburnus alburnus	N	S	p.a.	p.a.	7	nw	96 h	LC50	mortality	2300		Bengtsson *et al*. (1984)
Alburnus alburnus	N	S	-	7.8	7	-	96 h	LC50	mortality	2250-2400		Lindén *et al*. (1979)
Bacteria												
Vibrio fischeri	-	S	-	-	-	-	5 min	EC50	luminescence	3388		Cronin & Schultz (1997)
Vibrio fischeri	N	S	-	-	-	-	15 min	EC50	luminescence	2800		Hermens *et al*. (1985)
Vibrio fischeri	N	S	-	-	-	-	5 min	EC50	luminescence	3300		Bulich *et al*. (1981)
Vibrio fischeri	N	S	-	7.3	-	-	15 min	EC50	luminescence	2938		Gustavson *et al*. (1998)
CHRONIC TOXICITY-freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	875		Bringmann & Kühn (1979; 1980b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	650		Bringmann & Kühn (1976, 1977a, 1979, 1980b)

Species	Analysed	Test type	Substance purity	pH	Hardness Salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	100		Bringmann (1975), Bringmann & Kühn (1976)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	28		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	55		Bringmann (1978), Bringmann & Kühn (1979; 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	8.0		Bringmann & Kühn (1980a)

Notes
1: At 10 and 20 ºC.
2: At 30 ºC.

Table A1.2. Rejected toxicity data for 1-butanol.

Species	Analysed	Test type	Substance purity	pH	Hardness Salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Crustacea												
Daphnia magna	Y	S	>98%	-	-	-	48 h	LC50	mortality	16232	1	Pawlisz & Peters (1995)
ACUTE TOXICITY- saltwater												
Crustacea												
Elminius modestus	N	S	-	-	-	-	15 min	EC50	growth	0.038	2	Vaishnav & Korthals (1990)
Bacteria												
Vibrio fischeri	N	S			20	am	5 min	EC50	luminescence	44000	1	Chang *et al*. (1981)

Notes
1: Numbers are one order of magnitude higher than the rest.
2: This value is quoted from Crisp *et al.* (1967). In this paper values are expressed as thermodynamic activities, which are incorrectly recalculated to concentrations.

Table A1.3. Accepted toxicity data for 2-butanol.

Species	Analysed	Test type	Substance purity	pH	Hardness Salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	3400		Krebs (1991)
Crustacea												
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	3750		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	2300		Bringmann & Kühn (1982)
Daphnia magna, 6-24 h	N	Sc	-	8.0±0.2	240	am	48 h	EC50	immobility	4227		Kühn *et al*. (1989a)
Pisces												
Carassius auratus, 6.2±0.7 cm, 3.3±1.0 g	Y	S	-	7.8	283	tw	24 h	LC50	mortality	4300		Bridié *et al*. (1979)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	3520		Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	3540		Juhnke & Lüdemann (1978)
Pimephales promelas, 30 d, 18.9 mm, 0.090 g	Y	F	99%	7.82	44	-	96 h	LC50	mortality	3670		Geiger *et al*. (1986)
Amphibia												
Xenopus laevis, 3-4 w	N	S	Ag	8.0	200	DSW	48 h	LC50	mortality	1530		De Zwart & Slooff (1987)
CHRONIC TOXICITY-freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	95		Bringmann & Kühn (1979; 1980b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	500		Bringmann & Kühn (1976, 1977a, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	312		Bringmann (1975), Bringmann & Kühn (1976)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	745		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	1282		Bringmann (1978), Bringmann & Kühn (1979; 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	1416		Bringmann & Kühn (1980a)

Table A1.4. Accepted toxicity data for n-*butyl acetate.*

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY-freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	1200		Krebs (1991)
Crustacea												
Daphnia magna	-	-	-	-	-	-	24 h	EC50	immobility	24		Devillers *et al*. (1987)
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	205		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	205		Bringmann & Kühn (1982)
Pisces												
Danio rerio	N	S	-	7.5±0.3	-	-	96 h	LC50	mortality	62		Wellens (1982)
Lepomis macrochirus, 33-75 mm	N	S	Pure	7.6-7.9	55	nw	96 h	LC50	mortality	100		Dawson *et al*. (1975/1977)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	141		Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	71		Juhnke & Lüdemann (1978)
Pimephales promelas, 31-32 d, 21.6 mm, 0.175 g	Y	F	≥ 99%	7.2	43	-	96 h	LC50	mortality	18		Brooke *et al*. (1984)
ACUTE TOXICITY- saltwater												
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	32		Price *et al*. (1974)
Pisces												
Menidia beryllina, 40-100 mm	N	S	Pure	7.6-7.9	-	nw	96 h	LC50	mortality	185		Dawson *et al*. (1975/1977)
Bacteriophyta												
Vibrio fischeri	-	S	-	-	-	-	5 min	EC50	luminescence	70		Cronin & Schultz (1997)
CHRONIC TOXICITY-freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC10	O_2 production	600		Krebs (1991)
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	21		Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	115		Bringmann & Kühn (1976, 1977a, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	280		Bringmann (1975), Bringmann & Kühn (1976, 1978a,b)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	670		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	321		Bringmann (1978), Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	574		Bringmann & Kühn (1980a)

Table A1.5. Accepted toxicity data for cyclohexylamine.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	49	1	Krebs (1991)
Crustacea												
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	49	2,3	Bringmann & Kühn (1982)
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	80	2,4	Bringmann & Kühn (1977b)
Dapnhia magna	Y	-	-	-	-	-	24 h	EC50	immobility	58	2,5	Calamari *et al*. (1980)
Pisces												
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	58	1	Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	195	1	Juhnke & Lüdemann (1978)
Oncorhynchus mykiss	Y	-	-	7.4	320	-	96 h	LC50	mortality	90	2,6	Calamari *et al*. (1980)
CHRONIC TOXICITY- freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	0.32	2,7	Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	0.51	1	Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	420	1	Bringmann & Kühn (1976, 1977a, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	0.02	2,8	Bringmann (1975), Bringmann & Kühn (1976, 1978a,b)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	>400	1	Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	0.69	1	Bringmann (1978), Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	>200	1	Bringmann & Kühn (1980a)

Notes
1: pH adjusted before start of toxicity test.
2: pH not adjusted before start of toxicity test. Buffering capacity of test system unknown.
3: Test medium contains 1 mM HCO_3^-, which allows buffering of 0.5 mM cyclohexylamine (0.5 mM being the EC50).
4: Not buffered, not pH adjusted (chlorine free) tap water was used; unknown whether buffering capacity is sufficient.
5: Unknown whether buffering capacity in medium is sufficient.
6: Molar amount of CO_3^{2-} unknown, but due to higher hardness a higer buffering capacity is expected comared to the test result obtained at 20 mg/l $CaCO_3$.
7: An addition of 0.32 mg/l cyclohexylamine (0.32 mg/l being the NOEC) would increase the pH of a neutral aqueous solution to 8.5, which is considered acceptable.
8: An addition of 0.02 mg/l cyclohexylamine (0.02 mg/l being the NOEC) would increase the pH of a neutral aqueous solution to 7.5, which can not cause a pH effect.

Table A1.6. Rejected toxicity data for cyclohexylamine.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Selenastrum capricornutum	Y	S	ag	-	-	-	96 h	EC50	growth	20	1	Calamari *et al*. (1980)
Pisces												
Oncorhynchus mykiss	Y	-	-	7.4	20	-	96 h	LC50	mortality	44	1,2	Calamari *et al*. (1980)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	54	3	Yoshioka *et al*. (1986)
Danio rerio	N	S	-	-	-	-	96 h	LC50	mortality	470	1	Wellens (1982)
Protozoa												
Tetrahymena pyriformis	N	S	-	-	-	-	24 h	EC50	growth	210	3	Yoshioka *et al*. (1986)
CHRONIC TOXICITY- freshwater												
Bacteria												
Pseudomonas putida	N	Sc	-	-	81.2	am	16 h	NOEC	growth	10	1	Bringmann & Kühn (1976, 1977a, 1979, 1980b)

Notes

1: pH not adjusted before start of toxicity test. Buffering capacity of test system unknown.

2: Insufficient buffering capacity in medium; pH effect can not be ruled out, which is also mentioned by author.

3: Unknown whether buffering capacity in medium is sufficient.

Table A1.7. Accepted toxicity data for diethylene glycol.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Crustacea												
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	> 10000		Bringmann & Kühn (1982)
Daphnia magna	N	S	-	7.6-7.7	70	-	24 h	EC50	immobility	> 10000		Bringmann & Kühn (1977b)
Daphnia magna	Y	S	-	7.5-7.8	160-180	-	48 h	EC50	immobility	47200	1	Ward *et al*. (1992)
Pisces												
Carassius auratus, 6.2±0.7 cm, 3.3±1.0 g	Y	S	-	7.8	283	tw	24 h	LC50	mortality	>5000		Bridié *et al*. (1979)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	>10000		Juhnke & Lüdemann (1978)
Oncorhynchus mykiss, 0.64 g	Y	S	-	7.0-7.9	40-48	-	96 h	LC50	mortality	52800	1	Ward *et al*. (1999)
Oncorhynchus mykiss, 0.42 g	Y	S	-	7.7-8.3	-	-	96 h	LC50	mortality	62934	1	Beak Consultants (1995)
Pimephales promelas, 34 d, 0.102 g	Y	S	-	7.7	43.1	-	96 h	LC50	mortality	75200		Geiger *et al*. (1990)
Poecilia reticulata	-	S	-	-	25	-	168 h	LC50	mortality	61000		Könemann & Musch (1981)
Amphibia												
Xenopus leavis, 3-4 w	N	S	-	-	-	-	48 h	LC50	mortality	3065		De Zwart & Slooff (1987)
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	30030	2	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	39880	2	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	32480	2	Bantle *et al*. (1999)
Xenopus leavis, 3-4 w	Y	S	-	8.0-8.2	130-140	-	48 h	LC50	mortality	20358	1	Beak Consultants (1995)
Xenopus leavis, 3-4 w	Y	S	-	8.0-8.2	130-140	-	48 h	LC50	mortality	20496	1	Beak Consultants (1995)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	18740	2	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	17470	2	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	9740	2	Bantle *et al*. (1999)
Protozoa												
Tetrahymena pyriformis	N	S	>99%	-	-	am	36 h	EC50	growth	22500	3	Sauvant *et al*. (1995a)
Tetrahymena pyriformis	N	S	>99%	-	-	am	9 h	EC50	growth	24400	3	Sauvant *et al*. (1995a,b)
Tetrahymena pyriformis	N	S	>98%	-	-	-	9 h	EC50	growth	31500	3	Sauvant *et al*. (1995c)
ACUTE TOXICITY- saltwater												
Algae												
Skeletonema costatum	Y	S	-	8.1-8.2	-	-	96 h	EC50	growth	40800	1	Ward *et al*. (1992)
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	>10000	1	Price *et al*. (1974)
Mysidopsis bahia	Y	S	-	7.8-7.9	11.5-13.1	-	96 h	LC50	mortality	36900	1	Ward *et al*. (1992)
Pisces												
Cyprinodon variegatus	Y	S	-	7.6-7.9	11.5-16.8	-	96 h	LC50	mortality	62100	1	Ward *et al*. (1992)
Bacteriophyta												
Vibrio fischeri	N	S	-	-	-	-	15 min	EC50	luminescence	29000		Hermens *et al*. (1985)
CHRONIC TOXICITY-freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	2700		Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Bacteriophyta												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	8000		Bringmann & Kühn (1976, 1977a, 1979, 1980b)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	1700		Bringmann (1975), Bringmann & Kühn (1976, 1978a,b)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	>4000		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	10745		Bringmann (1978), Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	>8000		Bringmann & Kühn (1980a)

Notes

1: Data from Kent *et al*. (1999). Kent *et al*. is a review study which is considered a reliable source. Only acceptable data (Reliability 1 or 2) from Kent ***et al.*** are used.

2: Mean of three values tested in one laboratory.

3: inoculated with 10^4 - 5×10^4 cells/ml.

Table A1.8. Rejected toxicity data for diethylene glycol.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Pseudokirchneriella subcapitata	Y	S	-	7.4-7.6	-	-	72 h	EC50	growth	6400	1,2	Kent *et al*. (1999)
Pisces												
Gambusia affinis, adult female	N	S		7.8-8.5	-	nw	96 h	LC50	mortality	>32000	3	Wallen *et al*. (1957)

Notes

1: Algal test showed varying EC50 values: 6400 mg/l at 24 h, 24000 at 48 h, 6400 at 72 h and 19900 at 96 h. Test rejected because of this unexplained variability.

2: Data from Kent *et al*. (1999) are cited data. Kent *et al*. is a review study which is considered a reliable source. Only acceptable data (Reliability 1 or 2) from Kent *et al*. are used.

3: Turbidity 600-1500 mg/L.

Table A1.9. Accepted toxicity data for ethyl acetate.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY-freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	4300		Krebs (1991)
Scenedesmus subspicatus	N	S	-	8-9.3	-	-	48 h	EC50	biomass	3300		Kühn & Pattard (1990)
Scenedesmus subspicatus	N	S	-	8-9.3	-	-	48 h	EC50	growth rate	5600		Kühn & Pattard (1990)
Selenastrum sp.	-	-	-	-	-	-	96 h	EC50	growth	2500		Slooff (1982)
Crustacea												
Asellus aquaticus	N	S	>98%	-	-	-	48 h	LC50	mortality	1600		Slooff (1983)
Daphnia cucullata, 11 d	N	S	-	-	-	-	48 h	EC50	immobility	175	1	Canton & Adema (1978)
Daphnia cucullata, 11 d	N	S	-	-	-	-	48 h	EC50	immobility	154	1	Canton & Adema (1978)
Daphnia magna, <24 h	N	Sc	-	8.0±0.2	250	am	24 h	EC50	mortality	2306		Kühn *et al*. (1989b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	3090		Bringmann & Kühn (1982)
Daphnia magna, 24 h	N	S	-	7.6-7.7	70	-	24 h	EC50	immobility	2500		Bringmann & Kühn (1977b)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	660	1	Canton & Adema (1978)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	560	1	Canton & Adema (1978)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	819	1	Canton & Adema (1978)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	778	1	Canton & Adema (1978)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	698	1	Canton & Adema (1978)
Daphnia magna, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	786	1	Canton & Adema (1978)
Daphnia pulex, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	230	1	Canton & Adema (1978)
Daphnia pulex, < 1 d	N	S	-	-	-	-	48 h	EC50	immobility	295	1	Canton & Adema (1978)
Gammarus pulex	N	S	>98%	-	-	-	48 h	LC50	mortality	750		Slooff (1983)
Pisces												
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	270	1	Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	333	1	Juhnke & Lüdemann (1978)
Oncorhynchus mykiss, 5-8 w	N	S	>98%	7.8-8.0	272	tw	48 h	LC50	mortality	230		Slooff *et al*. (1983)
Oncorhynchus mykiss, 5-8 w	N	-	>98%	7-8		-	48 h	LC50	mortality	260		Slooff *et al*. (1983)
Oncorhynchus mykiss	N	R	-	-	-	-	96 h	LC50	mortality	484		Douglas *et al*. (1986)
Oncorhynchus mykiss	N	R	-	-	-	-	96 h	LC50	mortality	425		Douglas *et al*. (1986)
Oryzias latipes, 4-5 w	N	S	>98%	-	220	am	48 h	LC50	mortality	125	2	Slooff *et al*. (1983)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	1500	3	Tsuji *et al*. (1986)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	900	4	Tsuji *et al*. (1986)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	1500	5	Tsuji *et al*. (1986)
Pimephales promelas, 3-4 w	N	S	>98%	-	220	am	48 h	LC50	mortality	270		Slooff *et al*. (1983)
Pimephales promelas, 3-4 w	N	S				-	24 h	LC50	mortality	180-320		Slooff (1982)
Pimephales promelas, 29-30 d	Y	F	-	7.4	38	-	48 h	LC50	mortality	260		Call *et al*. (1981)
Pimephales promelas, 29-30 d	Y	F	>99%	7.4	38	-	96 h	LC50	mortality	230		Brooke *et al*. (1984)
Poecilia reticulata, 3-4 w	N	S	>98%	-	hard	am	48 h	LC50	mortality	210		Slooff *et al*. (1983)
Amphibia												
Ambystoma mexicanum, 3-4 w	N	S	-	-	220	am	48 h	LC50	mortality	150		Slooff & Baerselman (1980)
Xenopus laevis, 3-4 w	N	S	-	-	220	am	48 h	LC50	mortality	180		Slooff & Baerselman (1980)
Annelida												
Tubificidae	N	S	>98%	-	-	-	48 h	LC50	mortality	760		Slooff (1983)
Erpobdella octoculata	N	S	>98%	-	-	-	48 h	LC50	mortality	1200		Slooff (1983)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Coelenterata												
Hydra oligactis	N	S	>98%	-	220	am	48 h	LC50	mortality	1350		Slooff *et al*. (1983)
Insecta												
Aedes aegypti, 3th instar	N	S	>98%	-	220	am	48 h	LC50	mortality	350		Slooff *et al*. (1983)
Chironomus thummi	N	S	>98%	-	-	-	48 h	LC50	mortality	750		Slooff (1983)
Cloëon dipterum	N	S	>98%	-	-	-	48 h	LC50	mortality	480		Slooff (1983)
Corixa punctata	N	S	>98%	-	-	-	48 h	LC50	mortality	600		Slooff (1983)
Culex pipiens	N	S	>98%	-	220	am	48 h	LC50	mortality	3950		Slooff *et al*. (1983)
Ischnura elegans	N	S	>98%	-	-	-	48 h	LC50	mortality	600		Slooff (1983)
Nemoura cinerea	N	S	>98%	-	-	-	48 h	LC50	mortality	130		Slooff (1983)
Mollusca												
Lymnea stagnalis, 3-4 w	N	S	>98%	-	220	am	48 h	LC50	mortality	1100		Slooff *et al*. (1983)
Platyhelminthes												
Dugesia lugubris	N	S	>98%	-	-	-	48 h	LC50	mortality	3020		Slooff (1983)
Protozoa												
Tetrahymena thermophila	-	-	-	-	-	-	48 h	EC50	growth	100		Pauli *et al*. (1993)
Tetrahymena thermophila	-	-	-	-	-	-	48 h	EC50	growth	120		Pauli *et al*. (1993)
ACUTE TOXICITY- saltwater												
Bacteriophyta												
Vibrio fischeri	-	S	-	-	-	-	5 min	EC50	luminescence	5188		Cronin & Schultz (1997)
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	1590		Price *et al*. (1974)
Artemia salina, nauplii	Y	S	>98%	8.3-8.6	-	am	24 h	EC50	immobilisation	645	6	Foster & Tullis (1985)
Artemia salina, nauplii	Y	S	>98%	8.3-8.6	-	am	24 h	EC50	immobilisation	346	7	Foster & Tullis (1985)
CHRONIC TOXICITY-freshwater												
Algae												
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC10	O_2 production	1000		Krebs (1991)
Chlorella pyrenoidosa	N	S	>98%	-	-	am	48 h	NOEC	growth	>1000		Slooff *et al*. (1983)
Pseudokirchnerialla subcapitata	N	S	>98%	-	-	am	96 h	NOEC	growth	2000		Slooff *et al*. (1983)
Scenedesmus pannonicus	N	S	>98%	-	-	am	48 h	NOEC	growth	>1000		Slooff *et al*. (1983)
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	15		Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Crustacea												
Daphnia magna, <24 h	N	R	-	8.0±0.2	250	am	21 d	NOEC	mortality, reproduction	12	8	Kühn *et al*. (1989b)
Daphnia magna, <24 h	Y	R	-	8.0±0.2	250	am	21 d	NOEC	mortality, reproduction	2.4-12	8	Kühn *et al*. (1989b)
Bacteriophyta												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	650		Bringmann & Kühn (1976, 1977a, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	550		Bringmann (1975), Bringmann & Kühn (1976, 1978a,b)
Protozoa												
Tetrahymena thermophila	N	S	-	-	-	-	48 h	EC10	growth	20	9	Pauli *et al*. (1993)
Tetrahymena thermophila	N	S	-	-	-	-	48 h	NOEC	growth	12	9	Pauli *et al*. (1993)
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	3248		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	202		Bringmann (1978), Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	1620		Bringmann & Kühn (1980a)

Notes
1: results from different laboratory and different experiments
2: 24 ºC
3: 10 ºC
4: 20 ºC
5: 30 ºC
6: Test conducted in artifical sea water at 50% strength; no mortality in controls observed; 19°C.
7: Test conducted in artifical sea water at 25% strength; no mortality in controls observed; 19°C.
8: NOEC based on nominal value is 12 mg/l; 2.4 mg/l is the lowest measured concentration at this nominal concentration. The geometric mean of these two values (5.4 mg/l) will be used for ERL derivation.
9: 32 ºC; unknown whether these two endpoints result from independent tests. For ERL derivation, only the NOEC value will be used.

Table A1.10. Rejected toxicity data for ethyl acetate.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Protozoa												
Tetrahymena thermophila	N	S	-	-	-	-	1.5 h	EC10	movement	18		Pauli *et al*. (1994)

Table A1.11. Accepted toxicity data for ethylene glycol.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Pseudokircherniella subcapitata	Y	S	-	7.1-7.7	-		96 h	EC50	growth	5409	1	Aéroports de Montréal and Analex, Inc. (1994)
Crustacea												
Ceriodaphnia dubia, <24 h	N	S	-	8.1-8.7	160	-	48 h	EC50	immobility	29700	2	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	N	S	-	8.1-8.7	-	-	48 h	EC50	immobility	22600	2	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	N	S	-	8.1-8.7	-	-	48 h	EC50	immobility	25500	2	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	-	-	-	-	-	-	48 h	EC50	immobility	13900	3	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	-	-	-	-	-	-	48 h	EC50	immobility	10500	3	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	-	-	-	-	-	-	48 h	EC50	immobility	6900	3	Cowgill *et al*. (1985)
Ceriodaphnia dubia, <24 h	N	S	-	7.6-8.3	86	rw	48 h	LC50	mortality	34440		Pillard (1995)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	>10000		Bringmann & Kühn (1982)
Daphnia magna	N	S	-	7.6-7.7	70	-	24 h	EC50	immobility	>10000		Bringmann & Kühn (1977b)
Daphnia magna	N	S	-	-	-	-	24 h	EC50	immobility	74484	1	Calleja *et al*.(1994)
Daphnia magna	N	S	-	-	-	-	24 h	EC50	immobility	>10000		Conway *et al*. (1983)
Daphnia magna, < 24 h	N	S	-	8-8.6	-	-	48 h	EC50	immobility	51000	2	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8-8.6	-	-	48 h	EC50	immobility	41100	2	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8-8.6	-	-	48 h	EC50	immobility	47400	2	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8-8.6	-	-	48 h	EC50	immobility	46300	2	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8.2-8.5	-	-	48 h	EC50	immobility	57600	3	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8.2-8.5	-	-	48 h	EC50	immobility	45500	3	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8.2-8.5	-	-	48 h	EC50	immobility	51000	3	Cowgill *et al*. (1985)
Daphnia magna, < 24 h	N	S	-	8.2-8.5	-	-	48 h	EC50	immobility	51100	3	Cowgill *et al*. (1985)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Daphnia magna, neonates	N	S	rg	8.0	157	nw	48 h	LC50	mortality	46300		Gersich *et al*. (1986)
Daphnia magna	N	S	-	-	100	-	48 h	LC50	mortality	50450		Hermens *et al*. (1984)
Daphnia magna, <24 h	N	S	-	7.6	-	-	24 h	EC50	immobility	48582		Lilius *et al*. (1995)
Daphnia magna, < 24 h	N	S	-	7.6-7.9	160-180	-	48 h	LC50	mortality	54700		Ward *et al*. (1992)
Daphnia pulex	N	*S*	-	*7.6*	-	-	24 h	LC50	mortality	60406		Lilius *et al*. (1995)
Streptocephales proboscideus, 2^{nd}-3^{rd} instars	N	S	97->99%	-	-	-	24 h	LC50	mortality	54496		Calleja & Persoone (1992)
Procambarus sp., adult 13.6 g	N	S	99.9%	7.5	250-270	-	96 h	LC50	mortality	91430		Khoury *et al*. (1990)
Pisces												
Carassius auratus, 6.2±0.7 cm, 3.3±1.0 g	Y	S	-	7.8	283	tw	24 h	LC50	mortality	>5000		Bridié *et al*. (1979)
Lepomis macrochirus, 1.2 g	N	S	rg	7.1	44	-	96 h	LC50	mortality	>111400		Mayer & Ellersieck (1986)
Lepomis macrochirus, juvenile, 0.85 g	N	S	99.9%	7.5	250-270	-	96 h	LC50	mortality	27540		Khoury *et al*. (1990)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	>10000		Juhnke & Lüdemann (1978)
Oncorhynchus mykiss, 0.7 g	N	S	rg	7.4	44	-	96 h	LC50	mortality	45700		Mayer & Ellersieck (1986)
Oncorhynchus mykiss, 1.1 g	N	S	rg	7.4	44	-	96 h	LC50	mortality	17800		Mayer & Ellersieck (1986)
Oncorhynchus mykiss	N	-	rg	-	-	-	96 h	LC50	mortality	>18500		Jank *et al*. (1973)
Oncorhynchus mykiss, 0.7 g	N	S		7.2-7.5	40-50	-	96 h	LC50	mortality	41000		Jonhnson & Finley (1980)
Oncorhynchus mykiss, fry 60-90 d, 0.7 g	N	R	99%	7	-	-	96 h	LC50	mortality	56481		Greene & Kocan (1997)
Oncorhynchus mykiss, fry 60-90 d, 0.7 g	N	R	99%	7	-	-	96 h	LC50	mortality	60827		Greene & Kocan (1997)
Oncorhynchus mykiss, 4.2 cm	Y	S	-	7.8-8.3	-	-	96 h	LC50	mortality	22810	1	Beak Consultants Ltd (1995)
Oncorhynchus mykiss, 0.83 cm	Y	S	-	7.8-8.3	-	-	96 h	LC50	mortality	24591	1	Beak Consultants Ltd (1995)
Oncorhynchus mykiss, 0.7 g	N	S	-	7.2-7.5	40-50	-	96 h	LC50	mortality	41000	1	Johnson Finley (1980)
Oncorhynchus mykiss, 4.1 cm	Y	S	-	7.2-7.8	40-48	-	96 h	LC50	mortality	50800	1	Ward *et al* (1992)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	>1000	4	Tsuji *et al*. (1986)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	>1000	5	Tsuji *et al*. (1986)
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	mortality	>1000	6	Tsuji *et al*. (1986)
Pimephales promelas, fry 90-100 d, 0.1 g	N	R	99%	7	-	-	96 h	LC50	mortality	68275		Greene *et al*. (1997)
Pimephales promelas, fry 90-100 d, 0.1 g	N	R	99%	7	-	-	96 h	LC50	mortality	69516		Greene & Kocan (1997)
Pimephales promelas, fry 10-15 d	N	S	Tech	7.6-8.3	96-125	nw	96 h	LC50	mortality	53000		Mayes *et al*. (1983)
Pimephales promelas, juv. 30 d	N	S	Tech	7.6-8.3	96-125	nw	96 h	LC50	mortality	49000		Mayes *et al*. (1983)
Pimephales promelas, 60-100 d	N	S	Tech	7.6-8.3	96-125	nw	96 h	LC50	mortality	57000		Mayes *et al*. (1983)
Pimephales promelas	-	S	-	8.0-8.2	40-40	-	96 h	LC50	mortality	50400	1	Ward *et al* (1992)
Pimephales promelas	N	S	-	7.3-8.3	86	rw	96 h	LC50	mortality	72860	1	Pillard (1995)
Pimephales promelas	N	S	-	-	-	-	96 h	LC50	mortality	>10000		Conway *et al*. (1983)
Pimephales promelas	-	S	-	7.3-8.3	120-130	-	7 d	EC50	growth	37318	2	Beak Consultants Ltd (1995)
Pimephales promelas	-	S	-	7.3-8.3	120-130	-	7 d	LC50	mortality	47332	2	Beak Consultants Ltd (1995)
Poecilia reticulata	N	S	-	-	25	-	168 h	LC50	mortality	49300		Könemann & Musch (1981)
Amphibia												
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	20260	7	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	31000	7	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	LC50	mortality	28400	7	Bantle *et al*. (1999)
Xenopus laevis, 3-4 w	Y	S	-	7.8-8.1	120-140	-	48 h	LC50	mortality	15667	1	Beak Consultants Ltd (1995)
Xenopus laevis, 3-4 w	Y	S	-	7.8-8.1	120-140	-	48 h	LC50	mortality	19350	1	Beak Consultants Ltd (1995)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	12570	7	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	10470	7	Bantle *et al*. (1999)
Xenopus laevis	N	S	-	-	-	-	96 h	EC50	malformations	16610	7	Bantle *et al*. (1999)
Fungae												
Geotrichum candidum, geminated	N	-	-	6.5	-	-	4 h	EC50	glucose uptake	74482	8	Jacobsen (1995)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Insecta												
Chironomus tentans	N	S	-	-	-	-	10 d	LC50	mortality	15596	1	Aéroports de Montréal and Analex, Inc. (1995)
Macrophyta												
Lemna gibba	N	S	-	-	-	-	7 d	EC50	growth	10920	9	Barber *et al*. (1999)
Protozoa												
Tetrahymena pyriformis	N	S	>98%	-	-	am	9 h	EC50	growth	9400	10	Sauvant *et al*. (1995a,b)
Tetrahymena pyriformis	N	S	>98%	-	-	am	36 h	EC50	growth	13300		Sauvant *et al*. (1995a)
Tetrahymena pyriformis	N	S	>98%	-	-	am	9 h	EC50	growth	9300	10	Sauvant *et al*. (1995c)
Chilomonas paramaecium	N	S	-	8.0-8.2	-	-	48 h	LC50	mortality	53200	1	Ward & Boeri (1993)
Colpidium campylum	Y	S	-	-	-	-	24 h	EC50	growth	28090	1	Beak Consultants Ltd (1995)
Rotifera												
Brachionus calciflorus, post hatch	N	S	>99%	-	-	-	24 h	LC50	mortality	117930	11	Calleja & Persoone (1992), Calleja *et al*. (1994)
Brachionus calciflorus, 15-17 h	-	-	-	-	120-130	-	48 h	EC50	reproduction	26461	1	Beak Consultants Ltd (1995)
ACUTE TOXICITY- saltwater												
Algae												
Skeletonema costatum	Y	S	-	8.1-8.2	-	-	48 h	EC50	-	44200	1	Ward *et al*. (1992)
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	>20000		Price *et al*. (1974)
Artemia sp.	N	S	-	-	-	-	24 h	LC50	mortality	>20000		Conway *et al*. (1983)
Artemia salina	N	S	97-99%	-	35	-	24 h	LC50	mortality	180618	11	Calleja & Persoone (1992), Calleja *et al*. (1994)
Crangon crangon	N	R	-	-	-	-	96 h	LC50	mortality	50000		Blackman (1974)
Crangon crangon, adult	N	R	-	-	-	nw	48 h	LC50	mortality	>100	12	Portmann & Wilson (1971)
Mysidopsis bahia	Y	S	-	7.8-7.9	12.5-13.0	-	96 h	LC50	mortality	34200	1	Ward *et al*. (1992)
Pisces												
Cyprinodon variegatus	Y	S	-	7.2-7.5	10.0-14.7	-	96 h	LC50	mortality	27600	1	Ward *et al*. (1992)
Sciaenops ocellatus, tail bud 12-13h	N	S	-	-	30-32	am	40 h	EC50	hatching	167000	13	Robertson *et al*. (1988)
Sciaenops ocellatus, tail bud 12-13 h	N	S	-	-	30-32	am	40 h	EC50	mortality	145000	13	Robertson *et al*. (1988)
Rotifera												
Brachionus plicatilis, post hatch	N	S	>99%	-	15	-	24 h	LC50	mortality	149584		Calleja & Persoone (1992)
CHRONIC TOXICITY-freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	>10000		Bringmann & Kühn (1977a)
Crustacea												
Ceriodaphnia dubia, <24 h	N	S	-	7.3-8.2	86	rw	7 d	NOEC	mortality	24000		Pillard (1995)
Ceriodaphnia dubia, <24 h	-	*S*	-	7.3-8.2	86	rw	7 d	NOEC	reproduction	8590	14	Pillard (1995)
Ceriodaphnia dubia, <24 h	Y	S	-	7.5-8.2	120-130	-	7 d	NOEC	mortality	25957	1	Beak Consultants Ltd (1995)
Ceriodaphnia dubia, < 24 h	Y	*S*	-	7.5-8.2	120-130	-	7 d	NOEC	reproduction	3469	1	Beak Consultants Ltd (1995)
Pisces												
Oncorhynchus mykiss, sac fry, 10 d post hatch	Y	R	-	7.5-8.0	-	-	12-14 d	NOEC	growth	14692	1	Beak Consultants Ltd (1995)
Pimephales promelas, ≤ 7 d	Y	S	-	7.3-8.3	86	rw	7 d	NOEC	reproduction	15380	14	Pillard (1995)
Pimephales promelas, ≤ 7 d	Y	S	-	7.3-8.3	86	rw	7 d	NOEC	mortality	32000		Pillard (1995)
Pimephales promelas, ≤ 24 h	Y	R	-	7.4-8.25	120-130	-	7 d	NOEC	growth	12531	2	Beak Consultants Ltd (1995)
Pimephales promelas, ≤ 24 h	Y	R	-	7.4-8.25	120-130	-	7 d	NOEC	mortality	24569	2	Beak Consultants Ltd (1995)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	>10000		Bringmann & Kühn (1977a)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	2000		Bringmann & Kühn (1978b)
Insecta												
Chironomus tentans	N	S	-	-	-	-	10 d	NOEC	growth	4567	1	Aéroports de Montréal and Analex, Inc. (1995)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	112		Bringmann *et al*. (1980)
Chilomonas paramaecium	N	S	-	8.0-8.2	-	am	48 h	NOEC	mortality	40000	1	Ward & Boeri (1993)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	>10000		Bringmann (1978a)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	>10000		Bringmann & Kühn (1980b)
Rotifera												
Brachionus calyciflorus	Y	S	-	-	120-130	-	48 h	NOEC	reproduction	12800	1	Beak Consultants Ltd (1995)

Notes
1: Data cited from Kent *et al*. (1999). Kent *et al*. is a review study which is considered a reliable source. Only acceptable data (Reliability 1 or 2) from Kent *et al*. are used.
2: Tested at 20-21 °C.
3: Tested at 24-25 °C.
4: 10°C.
5: 20°C.
6: 30°C.
7: Mean of three values tested in one laboratory.
8: Strain ATCC 66592
9: Vegetative reproduction; changes in frond structure that may increase toxicant uptake and toxicity.
10: Inoculated with 10^4 - 5×10^4 cells/ml.
11 Data from Cajella *et al*. (1994) probably identical to data in Cajella & Persoone (1992).
12: Tested at 15 °C
13: EC50 was determined by linear interpolation between the highest and next to highest test concentration using logarithms of test concentrations.
14: endpoint reported as reproduction or growth.

Table A1.12. Rejected toxicity for ethylene glycol

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Pseudokirchneriella subcapitata	-	S	-	7.2-8.4	20-85	-	96 h	EC50		13067	1,2	Beak Consultants Ltd (1995)
Pseudokirchneriella subcapitata	Y	S	-	7.4-7.6	-	-	96 h	EC50		7900	1,3	Ward *et al*. (1992)
Crustacea												
Daphnia magna	-	-	-	-	-	-	48 h	LC50	mortality	18000	4	Lebkowska (1978)
Annelida												
Lumbriculus variegatus	-	-	-	-	-	-	48 h	LC50	mortality	37000	4	Lebkowska (1978)
Planorbarius corneus	-	-	-	-	-	-	96 h	LC50	mortality	47000	4	Lebkowska (1978)
Amphibia												
Rana brevipoda	-	-	-	-	-	-	48 h	LC50	mortality	17000	4	Nishiuchi (1984)
Xenopus laevis, 3-4 w	N	S	-	-	-	-	48 h	LC50	mortality	326	5	De Zwart & Slooff (1987)
Protozoa												
Paramecium caudatum	-	-	-	-	-	-	96 h	LC50	mortality	44000	4	Lebkowska (1978)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Vorticella microstoma	-	-	-	-	-	-	96 h	LC50	mortality	31000	4	Lebkowska (1978)
CHRONIC TOXICITY-freshwater												
Algae												
Pseudokirchneriella subcapitata	-	S	-	-	-	-	96 h	LOEC		20000	1,6	Pillard & DuFresne (1999)
Pseudokirchneriella subcapitata	-	S	-	7.2-8.4	20-85	-	96 h	NOEC		6963	1,2	Beak Consultants Ltd (1995)
Crustacea												
Ceriodaphnia dubia, ≤ 24 h	N	R	-	7.8-8.2	169	fw	7	MATC	mortality	4.2	7	Masters *et al*. (1991)
Ceriodaphnia dubia, ≤ 24 h	N	R	-	7.8-8.2	169	fw	7	MATC	reproduction	4.2	7	Masters *et al*. (1991)
Macrophyta												
Lemna minor	-	S	-	-	-	-	96 h	EC25	growth	10000	1,8	DuFresne & Pillard (1999)
Lemna minor	-	S	-	-	-	-	96 h	EC25	growth	17115	1,8	DuFresne & Pillard (1999)
Lemna minor	-	S	-	-	-	-	96 h	LOEC	growth	19848	1,6	DuFresne & Pillard (1999)
Lemna minor	-	S	-	-	-	-	96 h	LOEC	growth	20000	1,6	DuFresne & Pillard (1999)

1: Data cited from Kent *et al*. (1999). Kent *et al*. is a review study which is considered a reliable source. Only acceptable data (Reliability 1 or 2) from Kent *et al*. are used.
2: Classified as unacceptable in Kent *et al*. (1999).
3: Algal test showed varying EC50 values: <6400 mg/l at 24 h, 23100 at 48 h, <6400 at 72 h and 7900 at 96 h. Test rejected because of this unexplained variability.
4: Results are cited in GDCh (1991), the data originate from non-English studies, which can not be traced, and no additional information is given on test conditions and substance purity.
5: Value is a factor of 50 to 100 lower than the other two studies with the same species. The study is also designated as invalid in the review by Kent ***et al.*** (1999).
6: Since the percentage of effect found at the LOEC is not reported, a NOEC may not be derived from this LOEC (in compliance with TGD).
7: Study rejected because results were at least a factor of 1000 lower than all other results including chronic *C. dubia* studies. Study does report mg/l as unit for the result.
8. A NOEC can not be derived from an EC25 since the percentage of effect is >20 (in compliance with TGD).

Table A1.13. Accepted toxicity data for methanol.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Chlorella pyroneidosa	N	Sc	-	-	-	am	10-14 d	EC50	growth	28490	1	Stratton & Smith (1988)
Chlorella vulgaris	N	S	100%	-	-	am	96 h	EC50	growth	2610	6	El Jay (1996)
Chlorella zofingiensis	-	S	-	6.5	-	-	48 h	EC50	assimilation	7113		Weber *et al*. (1984)
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC50	O_2 production	12000		Krebs (1991)
Crustacea												
Assellus intermedius	N	S	-	6.5-8.5	130	nw	96 h	EC50	immobility	>100		Ewell *et al*. (1986)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	> 10000		Bringmann & Kühn (1982)
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	> 10000		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	>97%	-	-	-	24 h	EC50	immobility	21403		Calleja *et al*. (1994)
Daphnia magna, 1st and 2nd instar	N	R	-	6.5-8.5	130-	nw	96 h	LC50	mortality	>100		Ewell *et al*. (1986)
Daphnia magna, <24 h	-	S	>95%-	-	-	-	48 h	LC50	mortality	3289		Guilhermino *et al*. (2000)
Daphnia magna, 6-24 h	N	Sc	-	8.0±0.2	240	am	48 h	EC50	immobility	1983		Kühn *et al*. (1989a)
Daphnia magna, <24 h	N	S	-	7.6	-	-	24 h	EC50	immobility	20804		Lilius *et al*. (1995)
Daphnia magna, <24 h	N	S	-	7.7	154.5	nw	48 h	EC50	immobility	24500		Randall & Knopp (1980)
Daphnia magna	N	S	-	-	-	-	48 h	EC50	immobility	13240		Vaishnav & Korthals (1990)
Daphnia obtusa, <24 h	N	S	-	7.8-8.2	250	-	48 h	EC50	immobility	22200		Rossini & Ronco (1996)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Daphnia pulex, <24 h	N	S	pest.g.	-	-	dnw	18 h	LC50	mortality	19548		Bowman *et al*. (1981)
Daphnia pulex, <24 h	N	S	-	7.6	-	-	24 h	EC50	immobility	27468		Lilius *et al*. (1995)
Gammarus fasciatus	N	S	-	6.5-8.5	130	nw	96 h	EC50	immobility	>100		Ewell *et al*. (1986)
Hyalella azteca	N	S	pest.g.	-	-	dnw	18 h	LC50	mortality	19389		Bowman *et al*. (1981)
Streptocephalus proboscideus, 2nd-3rd instar	N	S	>97%	-	-	am	24 h	LC50	mortality	32681		Calleja & Persoone (1992), Calleja *et al*. (1994)
Pisces												
Lepomis macrochirus	Y	F	99%	-	-	-	72 h	LC50	mortality	17720		Call *et al*. (1983)
Lepomis macrochirus, juvenile 3.07 g	Y	F	-	7.04-7.97	46.6	nw	96 h	LC50	mortality	15400		Poirier *et al*. (1986)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	>10000		Juhnke & Lüdemann (1978)
Oncorhynchus mykiss, 0.8 g	N	S	Tech	7.4	44	-	96 h	LC50	mortality	15000		Mayer & Ellersieck (1986)
Oncorhynchus mykiss	Y	F	-	7.04-7.97	46.6	nw	96 h	LC50	mortality	20100		Poirier *et al*. (1986)
Oryzias latipes, 2 cm, 0.2 g	N	S	-	7.2	40	-	48	LC50	mortality	>10000	2	Tsuji (1986)
Oryzias latipes, 2 cm, 0.2 g	N	S	-	7.2	40	-	48	LC50	mortality	1400	3	Tsuji (1986)
Pimephales promelas	Y	F	-	-	-	-	72 h	LC50	mortality	28400		Call *et all*. (1983)
Pimephales promelas	N	S	-	6.5-8.5	130	nw	96 h	LC50	mortality	>100		Ewell *et al*. (1986)
Pimephales promelas, 28-32 d, 0.126 g	Y	F	-	7.04-7.97	46.6	nw	96 h	LC50	mortality	29400		Poirier *et al*. (1986)
Pimephales promelas, 0.12 g, 30 d	Y	F	-	7.5	45.5	nw	96 h	LC50	mortality	28100		Veith *et al*. (1983)
Poecilia reticulata, 2-3 mo	R	S	-	-	25	am	168 h	LC50	mortality	10860		Hermens & Leeuwangh (1982)
Annelida												
Lumbriculus variegatus	N	S	-	6.5-8.5	130	nw	96 h	EC50	immobility	>100		Ewell *et al*. (1986)
Bacteria												
Nitrosomonas sp.	N	Sc	-	6.5-8.0	-	am	24 h	EC50	NH_3 consumption	880		Blum & Speece (1991)
Cyanophyta												
Anabaena cylindrica	N	S	-	-	-	am	10-14 d	EC50	growth	20339	1	Stratton (1987)
Anabaena inaequalis	N	S	-	-	-	am	10-14 d	EC50	growth	21210	1	Stratton (1987)
Anabaena variabilis	N	S	-	-	-	am	10-14 d	EC50	growth	24771	1	Stratton (1987)
Anabaena sp.	N	S	-	-	-	am	10-14 d	EC50	growth	24692	1	Stratton (1987)
Nostoc sp.	N	S	-	-	-	am	10-14 d	EC50	growth	43369	1	Stratton (1987)
Fungae												
Geotrichum candidum, geminated	N	-	-	6.5	-	-	4 h	EC50	glucose uptake	48060	8	Jacobsen (1995)
Insecta												
Culex restuans, juvenile	N	S	pest.g.	-	-	dnw	18 h	LC50	mortality	20022		Bowman *et al*. (1981)
Mollusca												
Helioma trivolvis	N	S	-	6.5-8.5	130	nw	96 h	EC50	immobility	>100		Ewell *et al*. (1986)
Platyhelminthes												
Dugesia tigrina	N	S	-	6.5-8.5	130	nw	96 h	EC50	immobility	>100		Ewell *et al*. (1986)
Protozoa												
Paramecium caudatum	N	S	-	-	-	am	4 h	LC50	mortality	7690		Rajini *et al*. (1989)
Spirostomum ambiguum	N	S	-	7.4	2.8	am	24 h	EC50	development	17590		Naleęcz-Jawecki & Sawicki (1999)
Spirostomum ambiguum	N	S	-	7.4	2.8	am	24 h	LC50	mortality	36814		Naleęcz-Jawecki & Sawicki (1999)
Tetrahymena pyriformis, late log-phase	N	S	≥ 95%	-	-	am	48 h	EC50	growth	18756		Schultz *et al*. (1990), Schultz & Tichy (1993)
Rotifera												
Brachionus calyciflorus	N	S	>97%	-	-	am	24 h	LC50	mortality	35885		Calleja & Persoone (1992), Calleja *et al*. (1994)
ACUTE TOXICITY- saltwater												
Algae												
Chaetoceros calcitrans	N	S	rg	-	-	am	4 d	EC50	growth, AUC	13000	4	Okumura *et al*. (2001)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Dunaniella tertiolecta	N	S	rg	-	-	am	4 d	EC50	growth, AUC	18000	4	Okumura *et al*. (2001)
Eutreptiella sp.	N	S	rg	-	-	am	4 d	EC50	growth, AUC	180	4	Okumura *et al*. (2001)
Heterosigma akashiwo	N	S	rg	-	-	am	4 d	EC50	growth, AUC	180	4	Okumura *et al*. (2001)
Isochrysis galbana	N	S	rg	-	-	am	4 d	EC50	growth, AUC	17000	4	Okumura *et al*. (2001)
Pavlova lutheri	N	S	rg	-	-	am	4 d	EC50	growth, AUC	15000	4	Okumura *et al*. (2001)
Prorocentrum minimum	N	S	rg	-	-	am	4 d	EC50	growth, AUC	2600	4	Okumura *et al*. (2001)
Skeletonema costatum	N	S	rg	-	-	am	4 d	EC50	growth, AUC	6500	4	Okumura *et al*. (2001)
Tetraselmis tetrathele	N	S	rg	-	-	am	4 d	EC50	growth, AUC	22000	4	Okumura *et al*. (2001)
Crustacea												
Artemia salina, 24 h	N	S	-	-	35	am	24 h	LC50	mortality	1579		Barahona-Gomariz *et al*. (1994)
Artemia salina, 48 h	N	S	-	-	35	am	24 h	LC50	mortality	1101		Barahona-Gomariz *et al*. (1994)
Artemia salina, 72 h	N	S	-	-	35	am	24 h	LC50	mortality	901		Barahona-Gomariz *et al*. (1994)
Artemia salina, 2nd-3rd larval instar	N	S	>97%	-	-	am	24 h	LC50	mortality	43574		Calleja & Persoone (1992), Calleja *et al*. (1994)
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	>10000		Price *et al*. (1974)
Artemia salina, cyst	N	-	-	-	30	sw	48 h	EC50	growth	46778		Vismara (1998)
Artemia salina, cyst	N	-	-	-	30	sw	48 h	LC50	mortality	48060		Vismara (1998)
Crangon crangon, adult	N	R	-	-	-	nw	96 h	LC50	mortality	1345		Portmann & Wilson (1971)
Nitocra spinipes, adult, 4-6 w, 0.6-0.8 mm	N	S	pa	7.8-7.9	7	nw	96 h	LC50	mortality	12000		Linden *et al*. (1979), Bengtsson *et al*. (1984)
Palaemonetes kadiakensis, juvenile	N	S	pest.g.	-	-	dnw	18 h	LC50	mortality	21922		Bowman *et al*. (1981)
Pisces												
Agonus cataphractus, adult	N	R	-	-	-	nw	96 h	LC50	mortality	7914-26116		Portmann & Wilson (1971)
Alburnus alburnus	N	S	pa	7.8-7.9	7	nw	96 h	LC50	mortality	28000		Linden *et al*. (1979), Bengtsson *et al*. (1984)
Sciaenops ocellatus, tail bud 12-13 h	N	S	-	-	30-32	am	40 h	EC50	hatching	89000		Robertson *et al*. (1988)
Sciaenops ocellatus, tail bud 12-13 h	N	S	-	-	30-32	am	40 h	EC50	mortality	88000		Robertson *et al*. (1988)
Bacteria												
Vibrio fischeri	N	S	-	-	-	am	5-15 min	EC50	bioluminescence	29348		Calleja *et al*. (1994)
Vibrio fischeri	N	S	-	-	-	am	5 min	EC50	bioluminescence	125000		Curtis *et al*. (1982)
Vibrio fischeri	N	S	-	7.3	-	am	15 min	EC50	bioluminescence	58303		Gustavson *et al*. (1998)
Vibrio fischeri	N	S	-	-	-	am	15 min	EC50	bioluminescence	42000		Hermens *et al* (1985)
Vibrio fischeri	N	S	-	-	20	am	15 min	EC50	bioluminescence	14736		Schiewe *et al*. (1985)
Mollusca												
Cerastoderma edule, adult	N	R	-	-	-	nw	96 h	LC50	mortality	2612-7914		Portmann & Wilson (1971)
Mytilus edulis, 5-7 cm	Y	F	-	7.5-8.2	29-31	nw	96 h	LC50	mortality	15900, 15200, 16700	5	Helmstetter *et al*. (1996)
Rotifera												
Brachionus placitilis	N	S	>97%	-	15	am	24 h	LC50	mortality	51905		Calleja & Persoone (1992)
CHRONIC TOXICITY-freshwater												
Algae												
Chlorella vulgaris	N	S	100%	-	-	am	96 h	NOEC	growth	791		El Jay (1996)
Chlorella zofingiensis	N	S	-	6.5	-	-	48 h	NOEC	assimilation	801		Weber *et al*. (1984)
Chlorococcales mixed culture, exponential phase	N	Sc	-	-	-	am	24 h	EC10	O_2 production	1600		Krebs (1991)
Pseudokirchneriella subcapitata	N	S	100%	-	-	am	96 h	NOEC	growth	791		El Jay (1996)
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	8000		Bringmann & Kühn (1977)
Bacteriophyta												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	6600		Bringmann & Kühn (1977)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	530		Bringmann & Kühn (1978b)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	441		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	> 10000		Bringmann (1978a)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	> 10000		Bringmann & Kühn (1980b)
CHRONIC TOXICITY- saltwater												
Algae												
Chaetoceros calcitrans	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	4432	7	Okumura *et al*. (2001)
Dunaniella tertiolecta	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	7914	7	Okumura *et al*. (2001)
Eutreptiella sp.	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	19	7	Okumura *et al*. (2001)
Heterosigma akashiwo	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	56	7	Okumura *et al*. (2001)
Isochrysis galbana	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	6410	7	Okumura *et al*. (2001)
Pavlova lutheri	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	4511	7	Okumura *et al*. (2001)
Prorocentrum minimum	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	324	7	Okumura *et al*. (2001)
Skeletonema costatum	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	1108	7	Okumura *et al*. (2001)
Tetraselmis tetrathele	N	S	rg	-	-	am	4 d	NOEC	growth, AUC	11080	7	Okumura *et al*. (2001)
Bacteria												
Vibrio fischeri	Y	Sc	-	7±0.2	20	am	6±1 h	EC20	growth	8820		Gellert (2000)
Vibrio fischeri	Y	Sc	-	7±0.2	20	am	6±1 h	LOEC	growth	3990		Gellert (2000)

Notes

1: the period of testing is very long and unusual but cell growth and inhibition compared to control was determined every day during this period.

2: at 10 and 20 ^{o}C

3: at 30 ^{o}C

4: read from figure

5: closed vessels, at 16.3±0.9 ºC, LC50 values are an estimated value (50% mortality) and calculated with the trimmed Spearman-Karber method and the Inhibition Concentration Percentage method

6: determined from presented data with a log-logistic relationship

7: NOEC was determined by linear interpolation as EC0

Table A1.14. Rejected toxicity data for methanol.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Pisces												
Lepomis macrochirus	Y						96 h	LC50	mortality	15500	1	US EPA (1983)
Oncorhynchus mykiss, 0.8 g	N	S	-	7.2-7.5	40-50	-	96 h	LC50	mortality	19000	1	Johnson & Finley (1980)
Mollusca												
Anodonta imbecillis, juvenile	N	S	-	-	-	-	48 h	LC50	mortality	37	2	Keller (1993)
ACUTE TOXICITY- saltwater												
Algae												
Enteromorpha intestinalis	N	S	-	-	-	am	24 h	EC50	ion leakage	94005		Schild *et al*. (1995)
Cruestacea												
Artemia salina, cysts	N	S	-	-	30	am	48 h	EC10	growth	17401	3	Vismara, 1998
Artemia salina, cysts	N	S	-	-	30	am	48 h	EC10	mortality	27394	3	Vismara, 1998
Elminius modestus	N	S	-	-	-	-	15 min	EC50	growth	0.77	4	Vaishnav & Korthals (1990)
Bacteria												
Vibrio fischeri	-	-	-	-	-	-	4 h	EC50	bioluminescence	7690	5	Schiewe *et al*. (1985)
CHRONIC TOXICITY- freshwater												
Insecta												
Chironomus riparius	Y	Sc	99%	8.0	150	nw	96 h	NOEC	activity	10253		Van der Zandt *et al*. (1994)

Notes

1: results not used as the data originate from a study that is not available, probably duplicates of other studies

2: study was rejected because cited values were wrong by a factor of 1000. The study of Poirier *et al*. (1986) was cited but the number given for *Oncorhynchus mykiss* was the number for *Pimephales promelas* divided by a factor of 1000. A value for *Ceriodaphnia dubia* of 11 mg/L was also quoted but this species was not studied by Poirier *et al*. (1986).

3: EC10 values reconstructed with a log-logistic model from EC1, EC5, and EC50 values. In the paper, an EC1 is considered as NOEC. Data are not used, because the study is considered as an acute test.

4: This value is quoted from Crisp et al. (1967). In this paper values are expressed as thermodynamic activities, which are incorrectly recalculated to concentrations.

5: results not used due to deviating test duration. Value taken from EHC document. Value could not be found in original study.

Table A1.15. Accepted toxicity data for methyl ethyl ketone.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Crustacea												
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	8890		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	7060		Bringmann & Kühn (1982)
Daphnia magna, < 24 h	N	S	>80%	8	173		48 h	LC50	mortalilty	>520		LeBlanc (1980)
Daphnia magna, < 24 h	N	S	-	7.7	154.5	nw	48 h	EC50	immobility	5091		Randall & Knopp (1980)
Pisces												
Carassius auratius	N	S	-	-	-	fw	24 h	LC50	mortalilty	2400		Jensen (1978)
Lepomis macrochirus	N	S	-	6.9-7.5	84-163	fw	48 h	LC50	mortalilty	5640		Tumbull *et al*. (1954)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	4600		Juhnke & Lüdemann (1978)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	4880		Juhnke & Lüdemann (1978)
Pimephales promelas	Y	F	>99%	7.5	48	-	96 h	LC50	mortality	3220		Brooke *et al*. (1984)
Poecilia reticulata	N	S	-	-	25	-	24 h	LC50	mortality	5700		Dojlido (1979)
Protozoa												
Tetrahymena pyriformis	N	S	≥ 95%	-	-	-	48 h	EC50	growth	6000	1	Schultz *et al*. (1995)
ACUTE TOXICITY- saltwater												
Algae												
Skeletonema costatum	N	S	-	-	-	-	96 h	EC50	photosynthesis	>500		US EPA (1978)
Crustacea												
Americamysis bahia	-	-	-	-	-	-	96 h	LC50	mortality	>402		US EPA (1978)
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	1950		Price *et al*. (1974)
Pisces												
Cyprinodon variegatus	N	S	>80%	-	10-31	nw	96 h	LC50	mortality	>400		Heitmuller *et al*. (1981)
Bacteria												
Vibrio fischeri								EC50	bioluminescence	3886		Chen & Que Hee (1995)
Vibrio fischeri	-	-	-	-	-	-	-	EC50	bioluminescence	5050		Curtis *et al*. (1982)
CHRONIC TOXICITY-freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	4300		Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	1150		Bringmann & Kühn (1976, 1977a, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	120		Bringmann (1975), Bringmann & Kühn (1978a,b)
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	110		Bringmann & Kühn (1976)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	2982		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	190		Bringmann (1978), Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	2830		Bringmann & Kühn (1980a)

Notes

1: In the study by Schultz *et al*. (1995), the EC50 for tetrahymena is reported as 0.012 mM. However, from the data for –log EC50 (log EC50^{-1}) and the QSAR based on log K_{ow} for this parameter, it is evident that this number does not refer to the EC50 but to 1/EC50. The resulting value is in the same range as other toxicity data, including protozoans. The number of 0.012 mM (0.87 mg/L would be extremely small in comparison with the rest of the data.

Table A1.16. Rejected toxicity data for methyl ethyl ketone.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Pisces												
Gambusia affinis	-	-	-	7.8-8.3	-	nw	96 h	LC50	mortality	5600	1	Wallen *et al*. (1957)
Lepomis macrochirus	-	-	-	7.93	21	-	96 h	LC50	mortality	4467	2	Union Carbide Corp. (1980)

Notes

1: results not used as considered poorly reliable due to the use of unstandardised methods with turbid natural waters

2: results not used as the data originate from a study that is not available.

Table A1.17. Accepted toxicity data for tribromomethane.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Pseudokirchneriella subcapitata	N	-	-	-	-	-	96 h	EC50	chlorophyll	38.6		US EPA (1978)
Pseudokirchneriella subcapitata	N	-	-	-	-	-	96 h	EC50	growth rate	40.1		US EPA (1978)
Crustacea												
Daphnia magna, ≤24 h	N	S	≥80%	8.0	173	nw	48 h	LC50	mortality	46		LeBlanc, 1980
Daphnia pulex, 12 h	N	R				-	96 h	EC50	mortality	44		Trabalka & Burch (1978)
Pisces												
Cyprinus carpio, eggs	Y	R	-	-	120	nw	3-5 d	EC50	hatching, mortality	52	1	Mattice *et al*. (1981)
Cyprinus carpio, eggs	N	R	-	-	120	nw	3-5 d	EC50	hatching, mortality	76		Mattice *et al*. (1981)
Cyprinus carpio, eggs	N	R	-	-	110	am	3-5 d	EC50	hatching, mortality	80		Mattice *et al*. (1981)
Lepomis macrochirus, juv. 0.32-1.2 g	N	S	≥80%	6.7-7.8	32-34	-	96 h	LC50	mortality	29		Buccafusco *et al*. (1981)
ACUTE TOXICITY- saltwater												
Algae												
Skeletonema costatum	N	-	-	-	-	-	96 h	EC50	photosynthesis	12.3		US EPA (1978)
Crustacea												
Americamysis bahia	N	-	-	-	-	-	96 h	LC50	mortality	24.4		US EPA (1978)
Penaeus aztecus, 3.3 g	Y	F		8-8.5	25-35	nw	96 h	LC50	mortality	26		Anderson *et al*. (1979); Gibson *et al*. (1981)
Pisces												
Cyprinodon variegatus, 14-28 d, 8-15 mm	N	S	≥80%	-	10-31	nw	96 h	LC50	mortality	18		Heitmuller *et al*. (1981)
Cyprinodon variegatus, juv. <20 d	Y	IF	-	7.6-8.4	21-28	nw	96 h	LC50	mortality	7.1		Ward *et al*. (1981)
Brevoortia tyrannus, juv. 3.5 g	Y	F		8-8.5	25-35	nw	96 h	LC50	mortality	12		Anderson *et al*. (1979); Gibson *et al*. (1981)
Mollusca												
Crassostrea virginica, egg/larvae	Y	S	rg	-	25	nw	48 h	LC50	mortality	1.5	2	Stewart *et al*. (1979)
CHRONIC TOXICITY- fresh water												
Algae												
Pseudokirchneriella subcapitata	N	-	-	-	-	-	96 h	NOEC	chlorophyll	10		US EPA (1978)

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
salt water												
Pisces												
Cyprinodon variegatus, eggs	Y	IF	-	7.6-8.4	21-28	nw	28 d	NOEC	mortality	4.8		Ward *et al* (1981)

Notes
1: value corrected for toxicant decay.
2: LC50 is determined by a log-logistic dose response relationship from the presented data and corrected for the average actual concentration (42% of nominal) during the test. EC10 could not be determined reliable, but is probably lower than 0.05 mg/L. Study was cited in Posthumus *et al*. (1998) but not used, because no LC50 was given in the text.

Table A1.18. Accepted toxicity data for triethanolamine.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Algae												
Scenedesmus subspicatus	N	Sc	-	8.1-9.6	55	am	48 h	EC50	biomass	470		Kühn & Pattard (1990)
Scenedesmus subspicatus	N	Sc	-	8.1-9.6	55	am	48 h	EC50	growth rate	750		Kühn & Pattard (1990)
Crustacea												
Daphnia magna, <24 h, 0.315-0.630 mm	N	S	-	7.6-7.7	286	tw	24 h	EC50	immobility	1390		Bringmann & Kühn (1977b)
Daphnia magna, <24 h	N	S	-	8.0±0.2	250	am	24 h	EC50	immobility	1850		Bringmann & Kühn (1982)
Daphnia magna, <24 h	N	Sc	-	8.0±0.2	250	am	24 h	EC50	mortality	2038		Kühn *et al*. (1989b)
Pisces												
Carassius auratus, 6.2±0.7 cm, 3.3±1.0 g	Y	S	-	7.8	283	tw	24 h	LC50	mortality	>5000		Bridié *et al*. (1979)
Leuciscus idus melanotus	N	S	-	7-8	255	tw	48 h	LC50	mortality	>10000		Juhnke & Lüdemann (1978)
Pimephales promelas, 30 d, 18.1 mm, 0.083 g	Y	F	97%	7.8	-	-	96 h	LC50	mortality	11800		Geiger *et al* (1990)
CHRONIC TOXICITY- freshwater												
Algae												
Scenedesmus quadricauda	N	Sc	-	7.0	55	am	8 d	NOEC	growth	1.8	1	Bringmann & Kühn (1977a, 1978a,b, 1979, 1980b)
Scenedesmus quadricauda	N	Sc	-	-	55	am	8 d	NOEC	growth	715	2	Bringmann & Kühn (1978a,b)
Scenedesmus subspicatus	N	Sc	-	8.1-9.6	55	am	48 h	NOEC	biomass	62		Kühn & Pattard (1990)
Scenedesmus subspicatus	N	Sc	-	8.1-9.6	55	am	48 h	NOEC	growth rate	110		Kühn & Pattard (1990)
Crustacea												
Daphnia magna, <24 h	Y	R	-	8.0±0.2	250	am	21 d	NOEC	mortality	16	3	Kühn *et al*. (1989b)
Bacteria												
Pseudomonas putida	N	Sc	-	7.0	81.2	am	16 h	NOEC	growth	>10000	1	Bringmann & Kühn (1976, 1979, 1980b)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	7.0	55	am	8 d	NOEC	growth	47	1	Bringmann & Kühn (1976, 1978a,b)
Protozoa												
Chilomonas paramaecium	N	Sc	-	6.9	74.6	am	48 h	NOEC	growth	1768		Bringmann *et al*. (1980)
Entosiphon sulcatum	N	Sc	-	6.9	75.1	am	72 h	NOEC	growth	56		Bringmann (1978); Bringmann & Kühn (1979, 1980b)
Uronema parduczi	N	Sc	-	6.9	75.1	am	20 h	NOEC	growth	>10000		Bringmann & Kühn (1980a)

Notes
1: neutral
2: not neutralized, but a negative effect of increased pH is absent.
3: result expressed as nominal concentration, concentration loss was less than 20%

Table A1.19. Rejected toxicity data for ethanolamine.

Species	Analysed	Test type	Substance purity	pH	Hardness salinity*	Test water	Exposure time	Criterion	Endpoint	Value [mg/L]	Notes	Reference
ACUTE TOXICITY- freshwater												
Crustacea												
Ceriodaphnia dubia, < 24 h	N	S	-	-	-	dw	48 h	EC50	immobility	610	1	Warne & Schifko (1999)
ACUTE TOXICITY-saltwater												
Crustacea												
Artemia salina, nauplii <48 h	N	S	-	-	-	am	24 h	LC50	mortality	5600	1	Price *et al*. (1974)
Crangon crangon, adult	N	R	-	-	-	nw	48 h	LC50	mortality	>100	1	Portmann & Wilson (1971)
CHRONIC TOXICITY- freshwater												
Algae												
Chlorococcales mixed culture	N	Sc	-	-	-	am	24 h	EC10	O_2 production	>1000	1	Krebs (1991)
Scenedesmus subspicatus	N	S	-	-	-	-	72 h	NOEC		7.9	3	cited in IUCLID, European Commission (2000)
Scenedesmus subspicatus	N	S	-	-	-	-	72 h	NOEC		26	3	cited in IUCLID, European Commission (2000)
Bacteria												
Pseudomonas putida	N	Sc	-	-	81.2	am	16 h	NOEC	growth	>10000	3	Bringmann & Kühn (1977a)
Cyanophyta												
Microcystis aeruginosa	N	Sc	-	-	-	am	8 d	NOEC	growth	19	3	Bringmann & Kühn (1978a,b)

Notes
1: unkown whether the pH was adjusted or the buffer capacity of the system was sufficient.
2: not neutralized
3: Results not used as the data orginate from a study which is not available. Data for not neutralized solutions. Data for the neutralized substance are reported twice in IUCLID, however, with values differing by a factor of 10, e.g. 2.6 vs. 26 mg/L for EC10.

Appendix 2. Information on terrestrial toxicity

Legend

Species	species used in the test, if available followed by age, size, weight or life stage
Soil type	description of the used type of soil
o.m.	organic matter content of the soil
Clay	clay content of the soil
Temperature	temperature during exposure
Exposure time	h = hours, d = days, w = weeks, m = months, min. = minutes
Criterion	L(E)Cx = test result showing x% mortality (LCx) of effect (ECx). LC50s and EC50s are usually determined for acute effects, EC10s are for chronic effects; NOEC = no observed effect concentration, statistically determined
Result test soil	Concentration in the used test soil corresponding to the L(E)Cx or NOEC
Result standard soil	Concentration corresponding to the L(E)Cx or NOEC normalised to standard soil (containing 10% organic matter and 25% clay)

Contents

Table A2.1. Toxicity data of n-butyl acetate to terrestrial organisms.

Species	Species properties	Soil type	Purity [%]	pH	% o.m.	% clay	Temperature [°C]	Exposure time [d]	Criterion	Test endpoint	Result test soil [mg/kg$_{dw}$]	Result standard soil [mg/kg$_{dw}$]	Reference
ACUTE TOXICITY													
Macrophyta													
Lactuca sativa				7.8	1.4	12	20	14	EC50	growth	1459	7295	Adema & Henzen (1990)
CHRONIC TOXICITY													
Macrophyta													
Lactuca sativa				7.8	1.4	12	20	14	NOEC	growth	100	500	Adema & Henzen (1990)