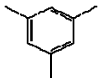
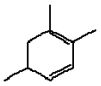
Summary report for 1,3,5-Trimetylbenzene (Mesitylene) and 1,2,4-Trimetylbenzene

SUMMARY

Substance name	**1,3,5-Trimetylbenzene and 1,2,4-Trimethylbenzene**			
CAS-number	**108-67-8 and 95-63-6**			
Proposed Quality Standard	**1,3,5-Trimetylbenzene**		**1,2,4-Trimethylbenzene**	
	Freshwater*			
	AA-QS	**MAC-QS**	**AA-QS**	**MAC-QS**
Water AF	**2 µg/L**	**20 µg/L**	**4 µg/L**	**43 µg/L**
Sediment	**/**	**/**	**/**	**/**
Remarks	**Harmonised proposal AA-QS 2 µg/L and MAC-QS 20 µg/L**			

*** marine and freshwater data**

1. IDENTITY

Substance name	1,3,5-Trimetylbenzene	1,2,4-Trimethylbenzene
CAS-number	108-67-8	95-63-6
Substance group	Organics	Organics
Synonyms	Mesitylene	/
Molecular formula	C_9H_{12}	C_9H_{12}
Structural formula		

2. PHYSICO-CHEMICAL PROPERTIES

Property	**1,3,5-Trimetylbenzene**	**1,2,4-Trimethylbenzene**	**ref.**
Molecular weight (g/mol)	120.1938	120.1938	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	280	280	SRC exp.
Water Solubility (mg/L)	48.2	57	SRC exp.
Log Kow	3.4	3.6	SRC exp.
Log Koc	2.8	2.9	SRC est.
Log K_{SED}	1.5	1.6	est. from K_{OC} - 5% OC
Henry-coefficient (Pa-m3/mol)	888	624	SRC exp.
pKa			

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic	**1,3,5-Trimetylbenzene**	**1,2,4-Trimethylbenzene**	**ref.**
BCF	86	125	SRC est.
(Aerobic bio)degradation	Readily biodegradable	Readily biodegradable	HSDB, SRC

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity 1,3,5-Trimetylbenzene (Mesitylene)

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Scenedesmus subspicatus (alg)	2d-EC50	39			RIVM database	2	F				
Invertebrates											
Daphnia magna (cru)			21d-NOEC	**0.4**	RIVM database	2	F		100		**4**
	2d-LC50	6			RIVM database	2	F				
Cancer magister (cru)	4d-LC50	**4.3**			RIVM database	1	M	100	1000	**43**	4.3
Artemia salina (cru)	1d-LC50	14			RIVM database	1	M				
Fish											
Carassius auratus (pis)	4d-LC50	12.5			RIVM database	1	F				

4.1 Aquatic acute and chronic toxicity 1,2,4-Trimetylbenzene

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
/											
Invertebrates											
Daphnia magna (cru)	2d-LC50	3.6			RIVM database	1	F				
Artemia salina (cru)	1d-LC50	12			RIVM database	1	M				
Cancer magister (cru)	4d-LC50	5.1			RIVM database	1	M				
Elasmopus pectinicrus (cru)	4d-LC50	4.4			RIVM database	1	M				
Palaemonetes pugio (cru)	4d-LC50	5.4			RIVM database	1	M				
Mysidopsis bahia (cru)	4d-LC50	**≈2.0**			IUCLID	1	M	100	1000	**20***	**2***
Fish											
Pimephales promelas (pis)	4d-LC50	7.7			RIVM database	1	F				

*** based on 2 trophic levels**

Summary report for 2-Methyl-4-isothiazolin-3-one

SUMMARY

Substance name	**2-Methyl-4-isothiazolin-3-one**			
CAS-number	**2682-20-4**			
Proposed Quality Standard	**Freshwater***			
	AA-QS	**MAC-QS**		
Water AF	**0.05 µg/L**	**0.5 µg/L**		
Sediment	**/**	**/**		
Remarks	**5-Chloro-2-methyl-4-isothiazolin-3-one AA-QS is 0.02 µg/L and MAC-QS is 0.22 µg/L**			

*** marine and freshwater data**

1. IDENTITY

Substance name	2-Methyl-4-isothiazolin-3-one
CAS-number	2682-20-4
Substance group	Organics
Synonyms	/
Molecular formula	C_4H_5NOS
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	115.1496	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	4.13	SRC est.
Water Solubility (mg/L)	536700	SRC est.
Log Kow	-0.8	SRC est.
Log Koc	1.4	SRC est.
Log K_{SED}	0.1	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	0.00089	SRC est.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	3	SRC est.
(Aerobic bio)degradation	Biodegradable	SRC

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Skeletonema costatum (alg)	3d-EC50	**0.05**			RIVM database	1	M	100	1000	**0.5**	**0.05**
Invertebrates											
Daphnia magna (cru)	2d-LC50	0.18			RIVM database	1	F				
Acartia tonsa (cru)	2d-LC50	0.056			RIVM database	1	M				
Fish											
Lepomis macrochirus (pis)	4d-LC50	0.3			RIVM database	1	F				
Oncorhynchus mykiss (pis)	4d-LC50	0.13			RIVM database	2	F				

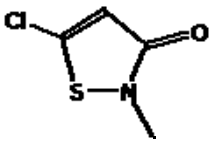
Summary report for 5-Chloro-2-methyl-4-isothiazolin-3-one

SUMMARY

Substance name	**5-Chloro-2-methyl-4-isothiazolin-3-one**			
CAS-number	**26172-55-4**			
Proposed Quality Standard	**Freshwater***			
	AA-QS	**MAC-QS**		
Water AF	**0.02 µg/L**	**0.22 µg/L**		
SSD	/	3.2 µg/L		
Sediment	**/**	**/**		
Remarks	**2-Methyl-4-isothiazolin-3-one AA-QS 0.05 µg/L and MAC-QS 0.5 µg/L**			

* marine and freshwater data

1. IDENTITY

Substance name	5-Chloro-2-methyl-4-isothiazolin-3-one
CAS-number	26172-55-4
Substance group	Organics
Synonyms	/
Molecular formula	C4H4ClNOS
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	149.5947	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	0.72	SRC est.
Water Solubility (mg/L)	148700	SRC est.
Log Kow	-0.3	SRC est.
Log Koc	1.6	SRC est.
Log K_{SED}	0.4	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	0.00072	SRC est.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	3	SRC est.
(Aerobic bio)degradation	Readily biodegradable	SRC

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Anabaena flosaquae (alg)	5d-EC50	0.29			RIVM database	1	F				
			5d-NOEC	0.25	IUCLID	1	F				
Selenastrum capricornutum (alg)	5d-EC50	**0.022**			RIVM database	1	F	100	1000	**0.22**	**0.02**
Skeletonema costatum (alg)	3d-EC50	0.036			RIVM database	2	M				
Invertebrates											
Ceriodaphnia dubia (cru)	2d-LC50	13			RIVM database	1	F				
Daphnia magna (cru)	2d-LC50	0.77			RIVM database	3	F				
			21d-NOEC	0.17	IUCLID	1	F		50		3.4**
Crassostrea virginica (mol)	2d-LC50	0.028			RIVM database	1	M				
Penaeus duorarum (cru)	4d-LC50	2.3			RIVM database	1	M				
Acartia tonsa (cru)	2d-LC50	0.56			RIVM database	1	M				
Uca pugilator (cru)	4d-LC50	59			RIVM database	1	M				
Fish											
Lepomis macrochirus (pis)	4d-LC50	1.1			RIVM database	3	F				
Oncorhynchus mykiss (pis)	14d-LC50	0.08			RIVM database	>3	F				
Cyprinodon variegatus (pis)	4d-LC50	0.36			RIVM database	1	M				
Other											
Lemna gibba (mac)			14d-EC50*	4.5	RIVM database	1	F				
Pseudomonas putida (bac)	16h-EC50	5.7			IUCLID	1	F				

*** additional chronic data**
**** rejected - not protective for all species**

Deriving MAC-QS: Acute EC50 → 9.6 µg/L (AF=3, 5 taxonomic groups from 3 trophic levels) → 3.2 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	0,29	alg-RIVM
2	0,022	alg-RIVM
3	0,036	alg-RIVM
4	13	cru-RIVM
5	0,77	cru-RIVM
6	0,028	mol-RIVM
7	2,3	cru-RIVM
8	59	cru-RIVM
9	0,56	cru-RIVM
10	1,1	pis-RIVM
11	0,08	pis-RIVM
12	0,36	pis-RIVM
13	5,7	bac-IUCLID
14		
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		
25		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-2,35E-1	mean of the log toxicity values
s.d.	1,06E0	sample standard deviation
n	1,30E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	8,832E-4	-3,054E0	lower estimate of the HC5
HC5	9,644E-3	-2,016E0	median estimate of the HC5
UL HC5	4,203E-2	-1,376E0	upper estimate of the HC5
sprHC5	4,758E1	1,677E0	spread of the HC5 estimate

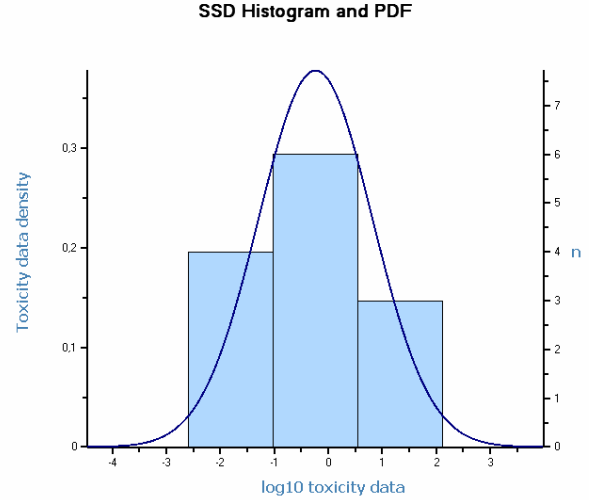
FA At HC5 results

Name	Value	Description
FA lower	0,85	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	17,30	95% confidence limit of the FA at standardised median logHC5

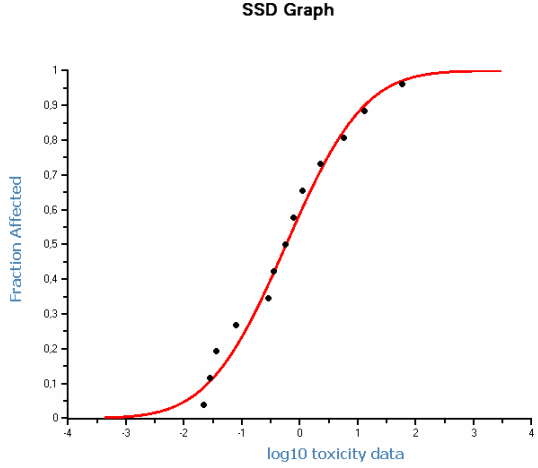
HC50 results

Name	Value	log10(Value)	Description
LL HC50	1,751E-1	-7,567E-1	lower estimate of the HC50
HC50	5,822E-1	-2,349E-1	median estimate of the HC50
UL HC50	1,936E0	2,869E-1	upper estimate of the HC50
sprHC50	1,106E1	1,044E0	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



Summary report for Antimony

SUMMARY

Substance name	**Antimony**	
CAS-number	**7440-36-0 (metal)**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	**3.2 µg/L**	**30 µg/L**
Sediment EP	**5.4 mg/kg dw + BC**	**51 mg/kg dw + BC**
Remarks	**Total RA for water. Added RA for sediment (lack of data for BC).**	

***data for fresh and marine water**

1. IDENTITY

Substance name	Antimony
CAS-number	7440-36-0
Substance group	Metals
Synonyms	/
Molecular formula	Sb
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	121.76	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	3.41(10% OC) → 3.23 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1 Aquatic toxicity data from RIVM database[a] and EPA Ecotox database[b]

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Skeletonema costatum	4d-EC50	> 4.15*			RIVM database	1	M				
Pseudokirchneriella subcapitata			4d-NOEC	0.20	EPA Ecotox	1	F				
Chlorella vulgaris			3-4d-NOEC	**0.032**	EPA Ecotox	1	F		10		**3.2**
Invertebrates											
Americamysis bahia (cru)	4d-LC50	> 4.15*			RIVM database	1	M				
Daphnia magna (cru)			7d-NOEC	3.9	EPA Ecotox	2	F				
Fish											
Oncorhynchus mykiss	28d-LC50	1.6 (from range)[c]			RIVM database	1	F				
Cyprinodon variegatus	4d-LC50	7.2 (from range)[c]			RIVM database	2	M				
Pimephales promelas			28d-NOEC	1.13	EPA Ecotox	1	F				
Other											
Gastrophryne carolinensis (amp)	7d-LC50	**0.3**			RIVM database	1	F	10		**30**	

a RIVM e-toxBase, Bilthoven, 2004
b http://www.epa.gov/ecotox/
c additional information

4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Ksed = 3.23
AA-QS sed = 1700 L/kg*0.0032 mg/L = 5.4 mg/ kg dw
MAC-QS sed = 1700 L/kg*0.030 mg/L = 51 mg/kg dw

Summary report for Arsenic

SUMMARY

Substance name		**Arsenic**	
CAS-number		**7440-38-2**	
Proposed Quality Standard		**Freshwater***	
		AA-QS	**MAC-QS**
Water	AF	0.33 µg/L	0.40 µg/L
	SSD	**7 µg/L + BC**	**21 µg/L + BC**
Sediment	**EP**	**31 mg/kg dw + BC**	**92 mg/kg dw + BC**
Remarks		**Added RA for water (BC = 1.4 µg/L) Added RA for sediment (lack of data for BC)**	

***data for fresh and marine water**

1. IDENTITY

Substance name	Arsenic
CAS-number	7440-38-2 (metal)
Substance group	Metals
Synonyms	/
Molecular formula	As
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	74.9216	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	3.82 (10% OC) → 3.644 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1.1 Aquatic toxicity data from RIVM database[a] and EPA Ecotox database[b]

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
/											
Invertebrates											
Ceriodaphnia reticulate (cru)	2d-EC50	1.8			RIVM database	1	F				
Daphnia magna (cru)	2d-EC50	3.8			RIVM database	1	F				
Daphnia pulex (cru)	2d-EC50	1.9			RIVM database	1	F				
Simocephalus vetulus (cru)	2d-EC50	1.7			RIVM database	1	F				
Acartia clause (cru)	4d-EC50	0.7			RIVM database	2	M				
Americamysis bahia (cru)	4d-EC50	2.0			RIVM database	2	M				
Americamysis bahia (cru)			51d-NOEC	0.6	RIVM database	1	M				
Purple sea urchin (ech)			2d-NOEC	**0.0033**[c]	EPA Ecotox	1	M		10		**0.33**
Fish											
Oncorhynchus mykiss	28d-LC50	1.6 (range)			RIVM database	1	F				
Carassius auratus	7d-LC50	0.49			RIVM database	1	F				
Pimephales promelas	4d-LC50	9.9			RIVM database	1	F				
Other											
Lemna minor (mac)			14d-NOEC	1.7	RIVM database	2	F				
Gastrophryne carolinensis (amp)	7 d-LC50	**0.04**			RIVM database	1	F	100		**0.40**	

a RIVM e-toxBase, Bilthoven, 2004
b http://www.epa.gov/ecotox/
c Lowest value of 20 NOEC data from 3 trophic levels (4.1.1 and 4.1.2)

4.1.2 Aquatic toxicity data from RIVM Report[a] (aggregated data) – chronic toxicity for freshwater and marine organisms

Table 5.1.1 Arsenic: freshwater data used for extrapolation

taxonomic group	NOEC in µg/l	taxonomic group	NOEC in µg/l
bac	9,700	cru	405[a]
cya	11,000	cru	88
alg	10	pis	2,100
alg	86	pis	2,100
alg	4,700	pis	76
alg	10,000	pis	8,400
pro	4,800	pis	1,900[b]
cru	570		

All data from Appendix I

a: most sensitive parameter(reproduction) for *D. magna*, geometric mean of 630 and 260 µg/l

b: most sensitive parameter(mortality/reproduction) for *P. promelas*, geometric mean of 1700 and 2100 µg/l

Table 5.1.2 Arsenic: marine data used for extrapolation

taxonomic group	NOEC (µg/l)
alg	95[a]
cru	630

All data from Appendix II

a: most sensitive parameter(reproduction) for *Champia parvula*

Species belonging to taxonomic group:
- bac = Bacteriophyta
- cya = Cyanophyta
- alg = Algae, not further classified
- mac = Macrophyta
- pro = Protozoa
- por = Porifera
- coe = Coelenterata
- mol = Mollusca
- nem = Nematoda
- ann = Annelida
- cru = Crustacea
- ins = Insecta
- ech = Echinodermata
- pis = Pisces
- amp = Amphibia

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

Deriving MAC-QS: HC5 = 0.104 mg/L (AF=5; 10 species from 3 major taxonomic groups from 2 trophic levels) → 20.8 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	1,8	cru-RIVM database
2	3,8	cru- RIVM database
3	1,9	cru- RIVM database
4	1,7	cru - RIVM database
5	0,7	cru - RIVM database
6	2	cru - RIVM database
7	1,6	pis - RIVM database
8	0,49	pis - RIVM database
9	9,9	pis - RIVM database
10	0,04	amp - RIVM database
11		
12		
13		
14		
15		
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17		
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19		
20		
21		
22		
23		
24		
25		
26		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	9,82E-2	mean of the log toxicity values
s.d.	6,35E-1	sample standard deviation
n	1,00E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	1,773E-2	-1,751E0	lower estimate of the HC5
HC5	1,040E-1	-9,829E-1	median estimate of the HC5
UL HC5	2,831E-1	-5,481E-1	upper estimate of the HC5
sprHC5	1,597E1	1,203E0	spread of the HC5 estimate

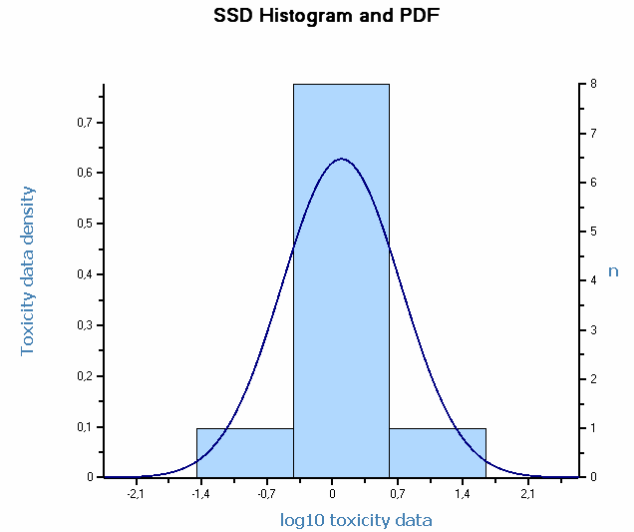
FA At HC5 results

Name	Value	Description
FA lower	0,61	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	20,04	95% confidence limit of the FA at standardised median logHC5

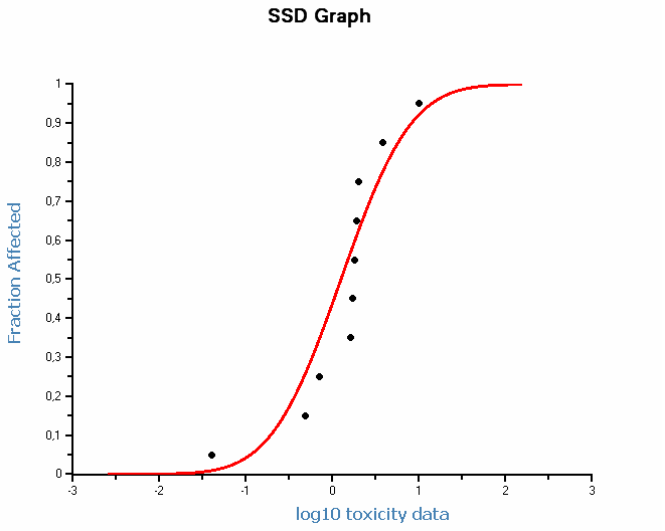
HC50 results

Name	Value	log10(Value)	Description
LL HC50	5,369E-1	-2,701E-1	lower estimate of the HC50
HC50	1,254E0	9,824E-2	median estimate of the HC50
UL HC50	2,928E0	4,666E-1	upper estimate of the HC50
sprHC50	5,453E0	7,366E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



Deriving AA-QS value: HC5=0.014 mg/L (AF=2; 20 species from 8 major taxonomic groups from 3 trophic levels) → 7 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	9,7	bac-INS
2	11	cya-INS
3	0,01	alg-INS
4	0,086	alg-INS
5	4,7	alg-INS
6	10	alg-INS
7	4,8	pro-INS
8	0,57	cru-INS
9	0,405	cru-INS
10	0,088	cru-INS
11	2,1	pis-INS
12	2,1	pis-INS
13	0,076	pis-INS
14	8,4	pis-INS
15	1,9	pis-INS
16	0,095	alg-marine-INS
17	0,63	cru-marine-INS
18	0,6	cru-RIVM database
19	1,7	mac-RIVM database
20	0,0033	coe-marine-EPA
21		
22		
23		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

Small sample

☐ Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-1,67E-1	mean of the log toxicity values
s.d.	1,02E0	sample standard deviation
n	2,00E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	2,502E-3	-2,602E0	lower estimate of the HC5
HC5	1,364E-2	-1,865E0	median estimate of the HC5
UL HC5	4,359E-2	-1,361E0	upper estimate of the HC5
sprHC5	1,742E1	1,241E0	spread of the HC5 estimate

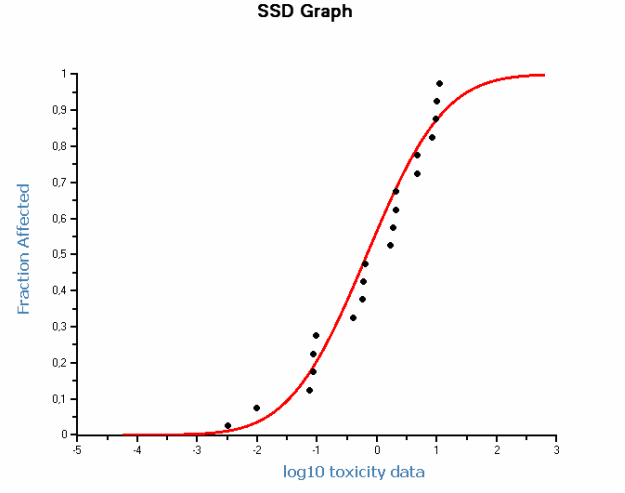
FA At HC5 results

Name	Value	Description
FA lower	1,28	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	13,98	95% confidence limit of the FA at standardised median logHC5

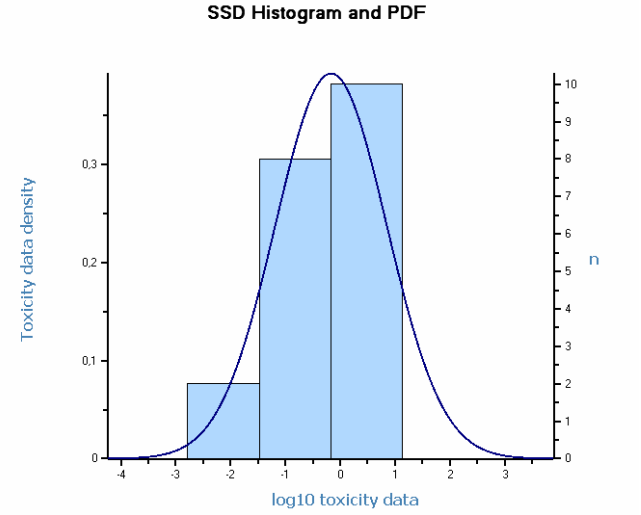
HC50 results

Name	Value	log10(Value)	Description
LL HC50	2,754E-1	-5,600E-1	lower estimate of the HC50
HC50	6,805E-1	-1,672E-1	median estimate of the HC50
UL HC50	1,681E0	2,257E-1	upper estimate of the HC50
sprHC50	6,106E0	7,857E-1	spread of the HC50 estimate

SSD graph



SSD Histogram and PDF



4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Ksed = 3.644
AA-QS sed = 4400 L/kg*0.007 mg/L = 30.8 mg/kg dw
MAC-QS sed = 4400 L/kg*0.0208 mg/L = 92 mg/kg dw

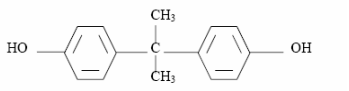
Summary report for Bisphenol-A

SUMMARY

Substance name	**Bisphenol-A**	
CAS-number	**80-05-7**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**1.6 µg/L**	**16 µg/L**
Sediment	**/**	**/**
Remarks	**EU RAR* data: AA-QS=PNEC (AF = 10) MAC-QS=PNEC*10**	

***** EU RISK ASSESSMENT Report, Final Report, 4,4'-ISOPROPYLIDENEDIPHENOL (BISPHENOL-A), 2003, United Kingdom (detailed evaluation of results - 1998 last full lit search, detailed searches until 2001)

1. IDENTITY

Substance name	Biphenol-A
CAS-number	80-05-7
Substance group	Organics
Synonyms	/
Molecular formula	$C_{15}H_{16}O_2$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	228.29	RAR
Vapour Pressure (Pa)	5.3E-06	RAR
Water Solubility (mg/L)	300	RAR
Log Kow	3.4	RAR
Log Koc	2.85	RAR
Log K_{SED}	1.55	est.from Koc -5%OC
Henry-coefficient (Pa-m3/mol)	0.000041	SRCest
pKa	/	/

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	67 (fish)	RAR
(Aerobic bio)degradation	Readily biodagradable	RAR

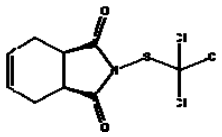
Summary report for Captan

SUMMARY

Substance name	**Captan**	
CAS-number	**133-06-2**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.1 µg/L***	**1.0 µg/L**
Sediment	**/**	**/**
Remarks	**data from dossier**	

*** Due to rapid degradation it is unlikely for the Captan to occur in water**

1. IDENTITY

Substance name	Captan
CAS-number	133-06-2
Substance group	Fungicide-Thiophthalimide
Synonyms	/
Molecular formula	$C_9H_8Cl_3NO_2S$
Structural formula	

Substance name	THPI**
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	THPAM**
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

**** Metabolite is not relevant due to the low toxicity**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**			**ref.**
Substance	Captan	THPI	THPAM	
Molecular weight (g/mol)	300.59	/	/	dossier
Vapour Pressure (Pa)	4.2E-06	/	/	dossier
Water Solubility (mg/L)	4.9	/	/	dossier
Log Kow	2.57	/	/	dossier
Log Koc	not measurable due to rapid hydrolysis	0.88-1.11	0.58-2.04 (pH dependent)	dossier
Log K_{SED}	/	/	/	/
Henry-coefficient (Pa-m3/mol)	3.0E-04	/	/	dossier
pKa	No	/	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic				**ref.**
Substance	Captan	THPI	THPAM	
BCF	140 (trigger value for readily degradable compounds is 1,000)	/	/	dossier
(Aerobic bio)degradation	Rapid hydrolytic degradation (days), likely to biodegrade very rapidly	/	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Captan

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	4d-EC50	1.6	(4d NOEC extrapolated)	(=1.18/3= 0.39)	PPP dossier	MS	F				
Daphnids											
Daphnia magna			21d-NOEC	0.56	PPP dossier	MS	F				
Fish											
Brown trout	4d-LC50	**0.098**			PPP dossier	MS	F	100	1000	**1**	**0.1**
Rainbow trout	4d-LC50	0.186			PPP dossier	MS	F				

4.1.2 Aquatic toxicity THPI

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	4d-EC50	> 180			PPP dossier	MS	F				
Daphnids											
Daphnia magna	2d-EC50	> 120			PPP dossier	MS	F				
Fish											
Rainbow trout	4d-LC50	> 12			PPP dossier	MS	F				

Aquatic toxicity of the metabolite THPI is between 10-100 mg/L → metabolite THPI is not relevant due to the low toxicity

4.1.3 Aquatic toxicity THPAM

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	4d-EC50	33			PPP dossier	MS	F				
Invertebrates											
Daphnia magna	2d-EC50	220			PPP dossier	MS	F				
Fish											
Rainbow trout	4d-LC50	> 12			PPP dossier	MS	F				

Aquatic toxicity of the metabolite THPAM is between 10-100 mg/L → metabolite THPAM is not relevant due to the low toxicity

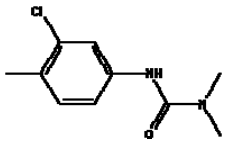
Summary report for Chlorotoluron

SUMMARY

Substance name	**Chlorotoluron**	
CAS-number	**15545-48-9**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water AF	**0.80 µg/L***	**8.0 µg/L***
Sediment	**/**	**/**
Remarks	**data from dossier**	

- **The sum of Chlorotoluron and Desmethyl chlorotoluron (the same mode of action)**

1. IDENTITY

Substance name	Chlorotoluron
CAS-number	15545-48-9
Substance group	Herbicide-Urea
Synonyms	/
Molecular formula	$C_{10}H_{13}ClN_2O$
Structural formula	

Substance name	3-(3-chloro-p-tolyl)1-methylurea
CAS-number	/
Substance group	Metabolite
Synonyms	Desmethyl chlorotoluron
Molecular formula	/
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**		**Ref.**
Substance	Chlorotoluron	Desmethyl chlorotoluron	
Molecular weight (g/mol)	212.7	/	dossier
Vapour Pressure (Pa)	5.0E-06	/	dossier
Water Solubility (mg/L)	74	/	dossier
Log Kow	2.5	/	dossier
Log Koc	2.0-2.6	2.28-2.51	dossier
Log K_{SED}	0.73-1.3	0.98-1.2	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	not determined due to very low vapour pressure	/	dossier
pKa	No	7	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic			**ref.**
Substance	Chlorotoluron	Desmethyl chlorotoluron	
BCF	Not relevant (log Kow=2.5)	/	dossier
(Aerobic bio)degradation	Not (bio)degradable	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Chlorotoluron

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	MAC-QS (µg/l)	AF AA-QS	AA-QS (µg/l)
Algae											
Scenodesmus subspicatus	3d-EC50	**0.024**	(3d-NOEC extrapolated)	**(=0.024/3=0.008)**	PPP dossier	MS	F	1	**8.0***	10	**0.80**
Daphnids											
Daphnia magna	2d-EC50	67	21d-NOEC	16.7	PPP dossier	MS	F				
Fish											
Rainbow trout	4d-LC50	20			PPP dossier	MS	F				
			21d-NOEC	0.4	PPP dossier	MS	F				
Aquatic plants											
Lemna gibba			7d-NOEC	**0.038**	PPP dossier	MS	F			10	3.8

*** MAC-QS derived from NOEC (AF = 1) is protective for algae, which are the most sensitive species**

4.1.2 Aquatic toxicity Desmethyl chlorotoluron

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	MAC-QS (µg/l)	AF AA-QS	AA-QS (µg/l)
Algae											
Scenodesmus subspicatus	3d-EC50	0.05			PPP dossier	MS	F				
Daphnids											
/											
Fish											
/											
Aquatic plants											
Lemna gibba			7d-NOEC	0.049	PPP dossier	MS	F				

From the toxicity data for Desmethyl chlortoluron it is obvious, that it has the same mode of action as Chlortoluron → toxicity unit approach is possible → the sum of both substances should not exceed QS

Summary report for Chromium

SUMMARY

Substance name		**Chromium**	
CAS-number		**7440-47-3**	
Proposed Quality Standard		**Freshwater***	
		AA-QS	**MAC-QS**
Water	AF	0.0058 µg/L	0.30 µg/L
	SSD	**12 µg/L + BC**	**160 µg/L + BC**
Sediment	**EP**	**1500 mg/kg dw**	**20400 mg/kg dw**
Remarks		**Added RA for water (BC = 3.4) Total RA for water**	

*** data for fresh and marine water**

1. IDENTITY

Substance name	Chromium
CAS-number	7440-47-3
Substance group	metals
Synonyms	/
Molecular formula	Cr
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	51.996	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	5.28 (10% OC) → 5.104 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1.1 Aquatic toxicity data from RIVM database[a] and EPA Ecotox database[b]

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Chlorella pyrenoidosa	4h-EC50	5			RIVM database	1	F				
Nitzschia palea	4h-EC50	0.8			RIVM database	1	F				
Chlorella protothecoides	3d-EC50	0.10			RIVM database	1	M				
Dunaliella tertiolecta (Green algae)	3d-EC50	17.4			RIVM database	2	M				
Gymnodinium splendens (Dinaflagellate)	2d-EC50	0.50			RIVM database	8	M				
Macrocystis pyrifera (Brown algae)	4d-EC50	5.0			RIVM database	1	M				
Selenastrum capricornutum (Green algae)	3d-EC50	0.50			RIVM database	1	M				
Thalassiosira guillardii (Diatom)	2d-EC50	0.79			RIVM database	10	M				
Gracilaria sp. (Red algae)			4d-NOEC	2.2	EPA Ecotox	1	M				
Gracilaria tenuistipitata (Red algae)			4d-NOEC	0.28	EPA Ecotox	2	M				
Pseudokirchneriella subcapitata (Green algae)			3d-NOEC	0.16	EPA Ecotox	4	M				
Invertebrates											
Aedes aegypti (ins)	2d-EC50	12.5			RIVM database	1	F				
Anodonta imbecillis (mol)	4d-EC50	0.16			RIVM database	2	F				
Brachionus calyciflorus (rot)	2d-EC50	8.3			RIVM database	1	F				
Ceriodaphnia reticulate (cru)	2d-EC50	0.045			RIVM database	1	F				
Chironomus sp (ins)	4d-EC50	11			RIVM database	1	F				
Cyclops sp (Copepoda- cru)	2d-EC50	10.5			RIVM database	1	F				
Daphnia ambigua (cru)	3d-EC50	3.6			RIVM database	2	F				
Daphnia galeata (cru)	3d-EC50	65.6			RIVM database	1	F				
Daphnia magna (cru)	3d-EC50	14.8			RIVM database	2	F				
Daphnia pulex (cru)	4d-EC50	90.4			RIVM database	1	F				
Daphnia pulicaria (cru)	3d-EC50	111			RIVM database	1	F				
Dugesia tigrina (cru)	4d-EC50	2.2			RIVM database	1	F				
Gammarus sp (Amphipoda - cru)	4d-EC50	3.2			RIVM database	1	F				
Lophopodella carteri (bry)	4d-EC50	1.6			RIVM database	1	F				
Pectinatella magnifica (bry)	4d-EC50	1.4			RIVM database	1	F				

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Plumatella emarginata (bry)	4d-EC50	0.65			RIVM database	1	F				
Scylla serrata (cru)	4d-EC50	56.3			RIVM database	1	F				
Simocephalus vetulus (cru)	2d-EC50	0.050			RIVM database	1	F				
Trichoptera (ins)	4d-EC50	50			RIVM database	1	F				
Zygoptera (ins)	4d-EC50	43.1			RIVM database	1	F				
Acartia clause (cru)	4d-EC50	6.6			RIVM database	1	M				
Americamysis bahia (cru)	4d-EC50	2.4			RIVM database	1	M				
Brachionus calyciflorus (rot)			2d-NOEC	2.0	RIVM database	1	F				
Americamysis bahia (cru)			51d-NOEC	0.088	RIVM database	1	M				
Artemia salina (cru)	2d-EC50	3.5			RIVM database	1	M				
Cerastoderma edule (mol)	2d-EC50	182			RIVM database	1	M				
Crangon crangon (cru)	2d-EC50	100			RIVM database	1	M				
Ophiothrix spiculata (ech)	7d-EC50	1.7			RIVM database	1	M				
Penaeus indicus (cru)	2d-EC50	1.0			RIVM database	1	M				
Perna viridis (mol)	2d-EC50	12.9			RIVM database	1	M				
Pseudodiaptomus coronatus (Copepod - cru)	4d-EC50	3.7			RIVM database	1	M				
Strongylocentrotus purpuratus (ech)			2d-NOEC	5.0	EPA Ecotox	1	M				
Acartia tonsa (Copepod - cru)			5d-NOEC	1.0	EPA Ecotox	1	M				
Fish											
Anguilla rostrata	4d-EC50	13.9			RIVM database	1	F				
Carassius auratus	7d-EC50	0.66			RIVM database	1	F				
Cyprinus carpio	4d-EC50	36.6			RIVM database	2	F				
Fundulus diaphanus	4d-EC50	16.9			RIVM database	1	F				
Lepomis gibbosus	4d-EC50	17			RIVM database	1	F				
Morone americana	4d-EC50	14.4			RIVM database	1	F				
Morone saxatilis	4d-EC50	17.7			RIVM database	1	F				
Mystus vittatus	4d-EC50	200			RIVM database	1	F				
Oncorhynchus mykiss	4d-EC50	100			RIVM database	1	F				
Pimephales promelas	4d-EC50	42.2			RIVM database	3	F				
Agonus cataphractus	2d-EC50	57.4			RIVM database	1	M				
Chrysiptera cyanea	4d-EC50	55.2			RIVM database	1	M				
Oryzias latipes	4d-EC50	157			RIVM database	3	M				
Pimephales promelas			7d-NOEC	2.0	RIVM database	1	F				

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Pimephales promelas			7d-NOEC	2.42	EPA Ecotox	13	F				
Other					RIVM database						
Amnicola (mac)	4d-EC50	10.2			RIVM database	2	F				
Lemna minor (mac)	4d-EC50	35			RIVM database	1	F				
Bufo melanostictus (Anura - amp)	4d-EC50	4.3			RIVM database	3	F				
Gastrophryne carolinensis (Anura - amp)	7d-EC50	**0.030**			RIVM database	1	F	100		**0.30**	

a RIVM e-toxBase, Bilthoven, 2004
b http://www.epa.gov/ecotox/

4.1.2 Aquatic toxicity data from RIVM Report[a] (aggregated data) – chronic toxicity for freshwater and marine organisms

Table 5.3.1 Chromium(VI): freshwater data used for extrapolation

taxonomic group	NOEC in µg/l	taxonomic group	NOEC in µg/l
bac	570[a]	coe	1,100
bac	380	rot	2,000
cya	83[b]	mol	110[h]
cya	3,300	cru	44[i]
alg	33[c]	cru	44[j]
alg	35	cru	20
alg	35	ins	1,100
alg	110[d]	pis	4,700[k]
alg	580	pis	290
alg	86[e]	pis	6,700[l]
alg	130[f]	pis	305[m]
mac	100	pis	520
mac	35[g]	pis	1,100[n]
mac	100	pis	100[o]
mac	100	pis	10
pro	0.058	pis	3,500[p]
pro	3,200	pis	1,000[q]
pro	9,600	pis	3,500[r]
pro	6,400	pis	100[s]
pro	1,000	pis	190[t]
pro	100	pis	110[u]
		amp	350[v]

AF (AA-QS) = 10 → AA-QS = 0.0058 µg/L

All data from Appendix I

a: geometric mean of 130 and 2500 µg/l, parameter mortality for *E. coli*
b: geometric mean of 1.9, 200, 200, 350, 110 and 110 µg/l, parameter growth for *M. aeruginosa*
c: lowest parameter(photosynthesis) for *C. pyrenoidosa*
d: geometric mean of 110 and 110 µg/l, parameter growth for *S. pannonicus*
e: geometric mean of 230 and 32 µg/l, parameter growth for *S. subspicatus*
f: geometric mean of 180, 110, 200 and 70 µg/l, parameter growth for *S. capricornutum*
g: geometric mean of 11 and 110 µg/l, parameter growth for *L. minor*
h: lowest parameter(reproduction) for *L. stagnalis*
i: lowest parameter(reproduction) for *C. dubia,* geometric mean of 32, 5.7, 65, 110 and 120 µg/l
j: lowest parameter(reproduction) for *D. magna,* geometric mean of 18, 270, 350, 35 and 2.9 µg/l
k: lowest parameter(growth) of the most sensitive life-stage(eggs) for *B. rerio*
l: lowest parameter(growth) for *G. aculeatus*
m: most sensitive life-stage(eggs)/parameter(growth) for *I. punctatus*
n: lowest parameter(growth) for *J. floridae*
o: lowest parameter(growth) of most sensitive life-stage(eggs) for *O. mykiss*, geometric mean of 200 and 51 µg/l
p: lowest parameter(mortality/growth) for *O. latipes*
q: lowest parameter(mortality) for *P. promelas,* geometric mean of 1000, 900 and 1100 µg/l
r: lowest parameter(growth) for *P. reticulata,* geometric mean of 3500 and 3500 µg/l
s: lowest parameter(growth) for *S. gairdneri,* geometric mean of 190 and 51 µg/l
t: lowest parameter(mortality/growth) for *S. fontinalis,* geometric mean of 100 and 350 µg/l
u: lowest parameter(growth) for *S. namaycush*
v: lowest parameter(mortality) for *X. laevis*

Species belonging to taxonomic group:

- bac = Bacteriophyta
- cya = Cyanophyta
- alg = Algae, not further classified
- mac = Macrophyta
- pro = Protozoa
- por = Porifera
- coe = Coelenterata
- mol = Mollusca
- nem = Nematoda
- ann = Annelida
- cru = Crustacea
- ins = Insecta
- ech = Echinodermata
- pis = Pisces
- amp = Amphibia

Table 5.3.2 Chromium(VI): marine data used for extrapolation

taxonomic group	NOEC in µg/l	taxonomic group	NOEC in µg/l
alg	402[a]	cru	88[d]
ann	50	cru	520[e]
ann	57[b]	cru	5,200[f]
ann	25[c]	cru	1,000
ann	500	cru	360
cru	770	cru	320

All data from Appendix II

a: geometric mean of 300, 600, 800, 1400, 350 and 60 µg/l, parameter growth for *S. costatum*

b: lowest parameter(reproduction) for *D. gyrociliatus*, geometric mean of 100 and 33 µg/l

c: lowest parameter(reproduction) for *N. arenaceodantata*

d: most sensitive life-stage for *M. bahia*, parameter(reproduction)

e: most sensitive parameter(reproduction) for *P. elegans*

f: geometric mean of 5200, 5200 and 5200 µg/l, parameter mortality for *P. varians*

Table 5.3.3 Chromium(III): freshwater data used for extrapolation

taxonomc group	NOEC in µg/l	taxonomic group	NOEC in µg/l
bac	1,300	cru	700
alg	100	pis	200
alg	100	pis	88[a]
alg	170		

All data from Appendix I

a: geometric mean of 48 and 160 µg/l, parameter mortality/growth/reproduction for *O. mykiss*

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

Deriving MAC-QS: HC5 = 0.16 mg/L (AF = 1; 54 species from 18 major taxononomic groups from 3 trophic levels) → 160 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	5	alg-RIVM
2	0,8	alg-RIVM
3	0,1	alg-Marine-RIVM
4	17,4	alg-Marine-RIVM
5	0,5	alg-Marine-RIVM
6	5	alg-Marine-RIVM
7	0,5	alg-Marine-RIVM
8	0,79	alg-Marine-RIVM
9	12,5	ins-RIVM
10	0,16	moll-RIVM
11	8,3	rot-RIVM
12	0,045	cru-RIVM
13	11	ins-RIVM
14	10,5	cru-RIVM
15	3,6	cru-RIVM
16	65,6	cru-RIVM
17	14,8	cru-RIVM
18	90,4	cru-RIVM
19	111	cru-RIVM
20	2,2	cru-RIVM
21	3,2	cru-RIVM
22	1,6	bry-RIVM
23	1,4	bry-RIVM
24	0,65	bry-RIVM
25	56,3	cru-RIVM
26	0,05	cru-RIVM

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Input toxicity data

Data no.	Toxicity data	Label
27	50	ins-RIVM
28	43,1	ins-RIVM
29	6,6	cru-RIVM
30	2,4	cru-RIVM
31	3,5	cru-Marine-RIVM
32	182	moll-Marine-RIVM
33	100	cru-Marine-RIVM
34	1,7	ech-Marine-RIVM
35	1	cru-Marine-RIVM
36	12,9	moll-Marine-RIVM
37	3,7	cru-Marine-RIVM
38	13,9	pis-RIVM
39	0,66	pis-RIVM
40	36,6	pis-RIVM
41	16,9	pis-RIVM
42	17	pis-RIVM
43	14,4	pis-RIVM
44	17,7	pis-RIVM
45	200	pis-RIVM
46	100	pis-RIVM
47	42,2	pis-RIVM
48	57,4	pis-Marine-RIVM
49	55,2	pis-Marine-RIVM
50	157	pis-Marine-RIVM
51	10,2	mac-RIVM
52	35	mac-RIVM

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Input toxicity data

Data no.	Toxicity data	Label
53	4,3	amp-RIVM
54	0,03	amp-RIVM
55		
56		
57		
58		
59		
60		
61		
62		
63		
64		
65		
66		
67		
68		
69		
70		
71		
72		
73		
74		
75		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	0,09E-1	mean of the log toxicity values
s.d.	9,64E-1	sample standard deviation
n	5,40E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	6,854E-2	-1,164E0	lower estimate of the HC5
HC5	1,637E-1	-7,859E-1	median estimate of the HC5
UL HC5	3,209E-1	-4,830E-1	upper estimate of the HC5
sprHC5	4,798E0	6,810E-1	spread of the HC5 estimate

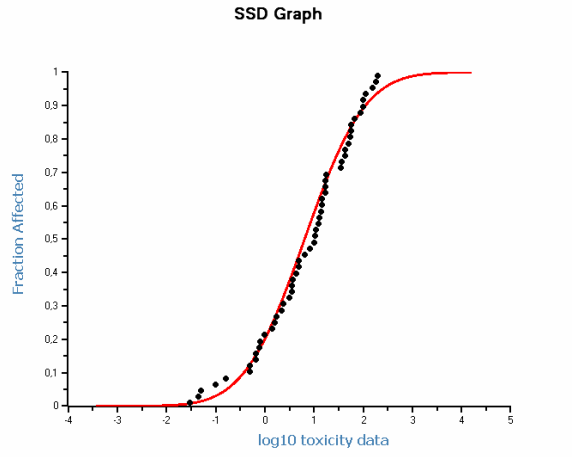
FA At HC5 results

Name	Value	Description
FA lower	2,28	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	8,04	95% confidence limit of the FA at standardised median logHC5

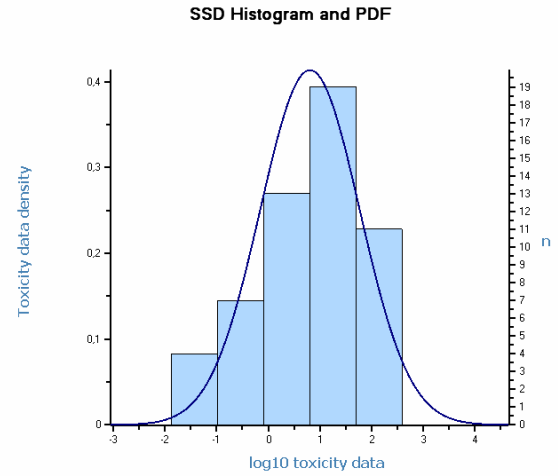
HC50 results

Name	Value	log10(Value)	Description
LL HC50	3,007E0	5,096E-1	lower estimate of the HC50
HC50	6,446E0	8,093E-1	median estimate of the HC50
UL HC50	1,069E1	1,029E0	upper estimate of the HC50
sprHC50	2,750E0	4,394E-1	spread of the HC50 estimate

SSD graph



SSD Histogram and PDF



Deriving AA-QS: HC5 = 0.012 mg/L (AF = 1; 71 species from 27 major taxonomic groups from 3 trophic levels) → 12 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	2,2	alg-marine-EPA
2	0,28	alg-marine-EPA
3	0,16	alg-marine-EPA
4	2	rot-RIVM
5	0,088	cru-marine-RIVM
6	5	ech-marine-EPA
7	1	cru-marine-EPA
8	2	pis-RIVM
9	2,4	pis-EPA
10	0,57	bac-INS
11	0,38	bac-INS
12	0,083	cya-INS
13	3,3	cya-INS
14	0,033	alg-INS
15	0,035	alg-INS
16	0,035	alg-INS
17	0,11	alg-INS
18	0,58	alg-INS
19	0,086	alg-INS
20	0,13	alg-INS
21	0,1	mac-INS
22	0,035	mac-INS
23	0,1	mac-INS
24	0,1	mac-INS
25	5,8E-05	pro-INS
26	3,2	pro-INS

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-5,28E-1	mean of the log toxicity values
s.d.	8,47E-1	sample standard deviation
n	7,10E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	6,161E-3	-2,210E0	lower estimate of the HC5
HC5	1,184E-2	-1,927E0	median estimate of the HC5
UL HC5	2,031E-2	-1,692E0	upper estimate of the HC5
sprHC5	3,296E0	5,180E-1	spread of the HC5 estimate

FA At HC5 results

Name	Value	Description
FA lower	2,50	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	7,46	95% confidence limit of the FA at standardised median logHC5

HC50 results

Name	Value	log10(Value)	Description
LL HC50	2,018E-1	-6,952E-1	lower estimate of the HC50
HC50	2,967E-1	-5,276E-1	median estimate of the HC50
UL HC50	4,364E-1	-3,601E-1	upper estimate of the HC50
sprHC50	2,163E0	3,350E-1	spread of the HC50 estimate

Input toxicity data

Data no.	Toxicity data	Label
27	9,6	pro-INS
28	6,4	pro-INS
29	1	pro-INS
30	0,1	pro-INS
31	1,1	coe-INS
32	2	rot-INS
33	0,11	mol-INS
34	0,044	cru-INS
35	0,044	cru-INS
36	0,02	cru-INS
37	1,1	ins-INS
38	4,7	pis-INS
39	0,29	pis-INS
40	6,7	pis-INS
41	0,305	pis-INS
42	0,52	pis-INS
43	1,1	pis-INS
44	0,1	pis-INS
45	0,01	pis-INS
46	3,5	pis-INS
47	1	pis-INS
48	3,5	pis-INS
49	0,1	pis-INS
50	0,19	pis-INS
51	0,11	pis-INS
52	0,35	amp-INS

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

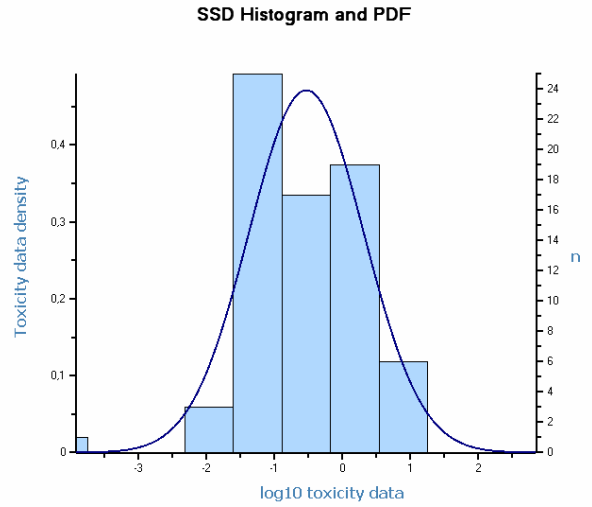
Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

SSD Histogram and PDF



Input toxicity data

Data no.	Toxicity data	Label
53	1,3	bac-INS(CrIII)
54	0,1	alg-INS(CrIII)
55	0,1	alg-INS(CrIII)
56	0,17	alg-INS(CrIII)
57	0,7	cru-INS(CrIII)
58	0,2	pis-INS(CrIII)
59	0,088	pis-INS(CrIII)
60	0,402	alg-marine-INS
61	0,05	ann-marine-INS
62	0,057	ann-marine-INS
63	0,025	ann-marine-INS
64	0,5	ann-marine-INS
65	0,77	cru-marine-INS
66	0,088	cru-marine-INS
67	0,52	cru-marine-INS
68	5,2	cru-marine-INS
69	1	cru-marine-INS
70	0,36	cru-marine-INS
71	0,32	cru-marine-INS
72		
73		
74		
75		
76		
77		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

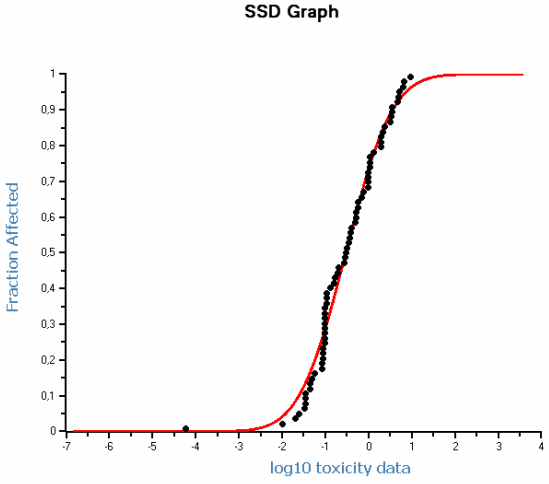
Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

SSD graph



4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Ksed = 5.104
AA-QS sed = 127057 L/kg*0.012 mg/L = 1520 mg/ kg dw
MAC-QS sed = 127057 L/kg*0.16 mg/L = 20400 mg/kg dw

Summary report for Cobalt

SUMMARY

Substance name	**Cobalt**	
CAS-number	**7740-48-4**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	**0.28 µg/L + BC**	**2.8 µg/L + BC**
Sediment EP	**0.74 mg/kg dw + BC**	**7.4 mg/kg dw + BC**
Remarks	**Added RA for water (lack of data for BC)** **Added RA for sediment (lack of data for BC)**	

*** marine and freshwater data**

1. IDENTITY

Substance name	Cobalt
CAS-number	7740-48-4
Substance group	metals
Synonyms	/
Molecular formula	Co
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	58.9332	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	3.60 (10% OC) → 3.424 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1 Aquatic toxicity data from RIVM database[a] and EPA Ecotox database[b]

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Chlorella vulgaris (Green algae)			3-4mon-NOEC	0.0042	EPA Ecotox	2	F				
Invertebrates											
Daphnia magna (cru)			28d-NOEC	**0.0028**	EPA Ecotox	>3	F	1	10	**2.8***	**0.28**
Ceriodaphnia dubia (cru)			7d-NOEC	0.050	EPA Ecotox	5	F				
Fish											
Carassius auratus	7d-EC50	0.81			RIVM database	1	F				
Oncorhynchus mykiss	28d-EC50	1.6[c]			RIVM database	>2	F				
Danio rerio			<4d-NOEC	3.84	EPA Ecotox	4	F				
Pimephales promelas			28d-NOEC	0.21	EPA Ecotox	9	F				
Other											
Gastrophryne carolinensis (Anura-amp)	7d-EC50	0.05			RIVM database	1	F	100		0.5	
Vibrio fischeri (bac)	30min-EC50	28.5			RIVM database	1	M				
Xenopus laevis (amp)			4d-NOEC	2.48	EPA Ecotox	1	F				

a RIVM e-toxBase, Bilthoven, 2004
b http://www.epa.gov/ecotox/
c MAC-QS derived from NOEC (AF = 1) is protective for all species

4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Ksed = 3.424
AA-QS sed = 2655 L/kg*0.00028 mg/L = 0.74 mg/ kg dw
MAC-QS sed = 2655 L/kg*0.0028 mg/L = 7.4 mg/kg dw

Summary report for Copper

SUMMARY

Substance name	**Copper**	
CAS-number	**7440-50-8**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water RAR max.bioavail. **RAR aver.bioavail.**	**8.2 µg/L** **30 µg/L**	**73 µg/L*** **290 µg/L***
Sediment	**98 mg/kg dw**	**548 mg/kg dw***
Remarks	**Water BC = 1 µg/L** **Sediment BC = 48 mg/kg dw**	

*** MAC-QS are derived linearly from the AA-QS: (AA-QS – BC) * 10 + BC**

1. IDENTITY

Substance name	Copper
CAS-number	7440-50-8
Substance group	Metals
Synonyms	/
Molecular formula	Cu
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	63.546	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	4.53 (10% OC) → 4.35 (5% OC) 4.39	a b
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997
b EU RAR Cu

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

An environmental risk assessment report (RAR) was produced by the European Copper Institute (ECI) [1]. There is a wealth of toxicity data that was systematically analysed and evaluated in the effects assessment section to derive a PNEC for use in the risk assessment. This document summarises their results.

The method for deriving the PNEC is the same as the method for the derivation of the AA-QS. Therefore it is proposed to use the PNECs presented in this report without any additional studies.

PNEC for freshwater
NOEC values were extracted from scientific publications and research activities. The database is extensive, so stringent selection criteria were applied to the extracted ecotoxicity data (e.g. only toxicity data with measured concentrations were used in the effects assessment), resulting in a final 'high quality' dataset of 123 individual chronic NOEC values from 22 different aquatic species. These species represent different trophic levels (primary producers, primary consumers and secondary consumers).

Chronic NOEC values are available for:

1. 3 unicellular algal species
   - *Raphidocelis subcapitata; Chlamydomonas reinhardtii; Chlorella vulgaris*
2. 1 higher plant
   - *Lemna minor*
3. 3 insect species
   - *Clistoronia magnifica; Chironomus riparius; Paratanytarsus parthenogeneticus*
4. 2 mollusc species
   - *Juga plicifera, Campeloma decisum*
5. 5 crustacean species
   - *Ceriodaphnia dubia; Daphnia magna; Daphnia pulex; Hyalella azteca; Gammarus pulex*
6. 8 fish species
   - *Pimephales notatus; Pimephales promelas; Oncorhynchus mykiss; Oncorhynchus kisutch; Ictalurus punctatus; Perca fluviatilis; Salvelinus fontanilis; Noemacheilus barbatulus.*

It was considered that both the added and the background copper concentrations may contribute to the observed effects and therefore the total risk approach was implemented.

Selection of data and analysis of the variations

[1] European Copper Institute:
CAS No: 7440-50-8, 7758-98-7, 1317-3-1, 1317–38–0, 1332-65-6 (EINECS No: 231–159–6, 231–847–6, 215-270-7, 215–269–1, 215-572-9) : Summary voluntary risk assessment report on copper, copper II sulphate pentahydrate, copper(i)oxide, copper(II)oxide, dicopper chloride trihydroxide, Based on draft report of 15 May 2005

Large variations in the results per species were observed, which were explained by a difference in bioavailability of Cu. Chronic Biotoc Ligand Models (BLM) were developed for algae (*P. subcapitata*), invertebrates (*D. magna*) and fish (*O. mykiss* and *P. promelas*). This model provided a mechanistic basis for understanding the bioavailability by integrating the chemical parameters (e.g., pH, hardness, DOC) and biological parameters (receptor sites on organism, mode of action).
These BLMs were used to normalise the individual NOECs to a predefined standard medium representative for the EU surface waters, thus producing a generic PNEC. Two scenarios were considered:

- a reasonable worst case scenario ($PNEC_{generic,rwc}$) with maximised bioavailability of Cu to the freshwater organisms:
  - 10^{th} percentile of hardness and DOC for all organisms (i.e. respectively 37 mg/l CaCO3 and 2.6 mg/l);
  - 10^{th} percentile of pH for invertebrates and fish (i.e. 6.6); 90th percentile of pH for algae (i.e. 8.1)
- a typical scenario ($PNEC_{generic,typical}$) with an 'average' bioavailability of Cu to the freshwater organisms, environmental:
  - 50^{th} percentile of hardness, pH and DOC for all organisms (i.e. respectively 99 mg/l CaCO3, 7.5 and 6.4 mg/l).

The data were aggregated according to the descriptions in the TGD (EC 2003) and the statistical extrapolation method (species Sensitivity Distributions SSD) was applied using the NOEC data that were corrected for bioavailability. The median 5^{th}-percentile of this distribution resulted in:

- **$HC5_{generic,rwc}$ = 8.2 µg/l** (total dissolved, maximising bioavailability) and
- **$HC5_{generic,typical}$ = 30.3 µg/l** for typical (average) bioavailability conditions

Due to the nature and extent of the available data, no additional assessment factor was applied (AF = 1).

Validation against background levels of Copper

The proposed PNEC for the aquatic compartment (surface waters) was validated by comparing with copper background levels, the optimal concentration ranges, and the essentiality levels. That analysis shows that the total dissolved PNEC-value is close to the copper background range (0.8 – 5 µg Cu/l) and falls within the optimal concentration range, determined from toxicity/deficiency experiments (1-35 µg Cu/l) and within the optimal concentration ranges as determined for the energy reserve of *D. magna* after acclimation 1-12 µg Cu/l.

PNEC for benthic organisms

Also for benthic organisms a large number of tests were available and the application of stringent quality criteria resulted in a final 'high quality' dataset of 106 individual chronic NOEC values for 6 different sediment-dwelling organisms i.e. the ampiphod *Hyalella azteca* (25 individual NOEC values) and *Gammarus pulex* (6 individual NOEC values), the oligochaete *Tubifex tubifex* (39 individual NOEC values) and *Lumbriculus variegatus* (3 individual NOEC values), the insect *Chironomus riparius* (27 individual NOEC values) and the insect *Hexagenia* (6 NOEC values). The selected NOEC range of the non-normalized data ranged between 18.3 mg/kg dry wt. and >3,158 mg/kg. dry wt. (min-max value).

The intraspecies sensitivity was further evaluated. Organic carbon and the Acid Volatile Sulfide[2] pool controlled the chronic toxicity of Cu towards sediment-dwelling organisms:

- Increasing AVS concentrations increased the EC_{10} values (and EC_{50}) (i.e. sediments becoming less toxic due to the unavailability of sulphide bound copper), and
- An almost linear positive relationship was observed between the toxicity values and the organic carbon content of the sediment.

Thus it was decided that a correction for bioavailability was to be made. Only NOEC data generated in oxic sediments (with low AVS) were retained. Thus the original dataset containing 106 NOEC values was trimmed to a data set of 62 NOEC values for copper. These retained NOEC values were normalized for organic carbon content using the following formula:

$$NOEC_{OC,\ normalized} = \frac{NOEC_{total}}{fOC}$$

with:

$NOEC_{total}$ *(mg Cu/kg dry wt.)*

fOC = fraction organic carbon;

$NOEC_{OC,\ normalized}$ *(mg/g OC)*

Thus $PNEC_{freshwater,oxic\ sediment}$ is based on the organic carbon normalized dataset, containing only low AVS sediments. Since the data sets is relatively large (6 data points representing 62 NOEC values screened to be representative of reasonable worst case conditions (low AVS levels)) PNEC was derived by SSD.

HC_5 was 30.9 µmol/gOC = 1,961 µg Cu/gOC.

Using a weight fraction of 0.05 organic carbon (kg Oc/kg solid) for a standard EU sediment (cfr TGD 2003), this value was converted to a **PNEC of 98 mg Cu/dry wt standard sediment**.

This value was validated against the sensitivity of benthic species in 'water-only exposure'. It was concluded that benthic species are not more sensitive than pelagic species, thus the PNEC water of 8.2 ug/L is protective for benthic organisms.

PNEC oxic sediment can be used for aerobic sediments. For **anaerobic** sediments both the amount of AVS and organic carbon in the sediment will influence the bioavailability and normalisation for OC as well as correction for AVS is required.

[2] Acid volatile sulfide (AVS) is an operational defined parameter indicating those sulfides, which are readily extracted by the cold extraction of sediment in approximately 1 M HCl acid.

Summary report for Cyanide

SUMMARY

Substance name	**Cyanide**	
CAS-number	57-12-5	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	0.43 µg/L	0.49 µg/L
SSD	**1.2 µg/L**	**17 µg/L**
Sediment	**/**	**/**
Remarks	**SSD method was selected due to the large number of data**	

*** data for marine and freshwater**

1. IDENTITY

Substance name	Cyanide
CAS-number	57-12-5
Substance group	Inorganics
Synonyms	/
Molecular formula	CN^--
Structural formula	$-C \equiv N^-$

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	26.02	Chemifinder
Vapour Pressure (Pa)	9.89E+04	SRC exp.
Water Solubility (mg/L)	1E+06	SRC exp.
Log Kow	-0.25	SRC exp.
Log Koc	0.43	SRC
Log K_{SED}	-0.87	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	13.5	SRC exp.
pKa	/	/

* http://chemfinder.cambridgesoft.com/

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	3.2	SRC est.
(Aerobic bio)degradation	Readily biodegradable	SRC

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity

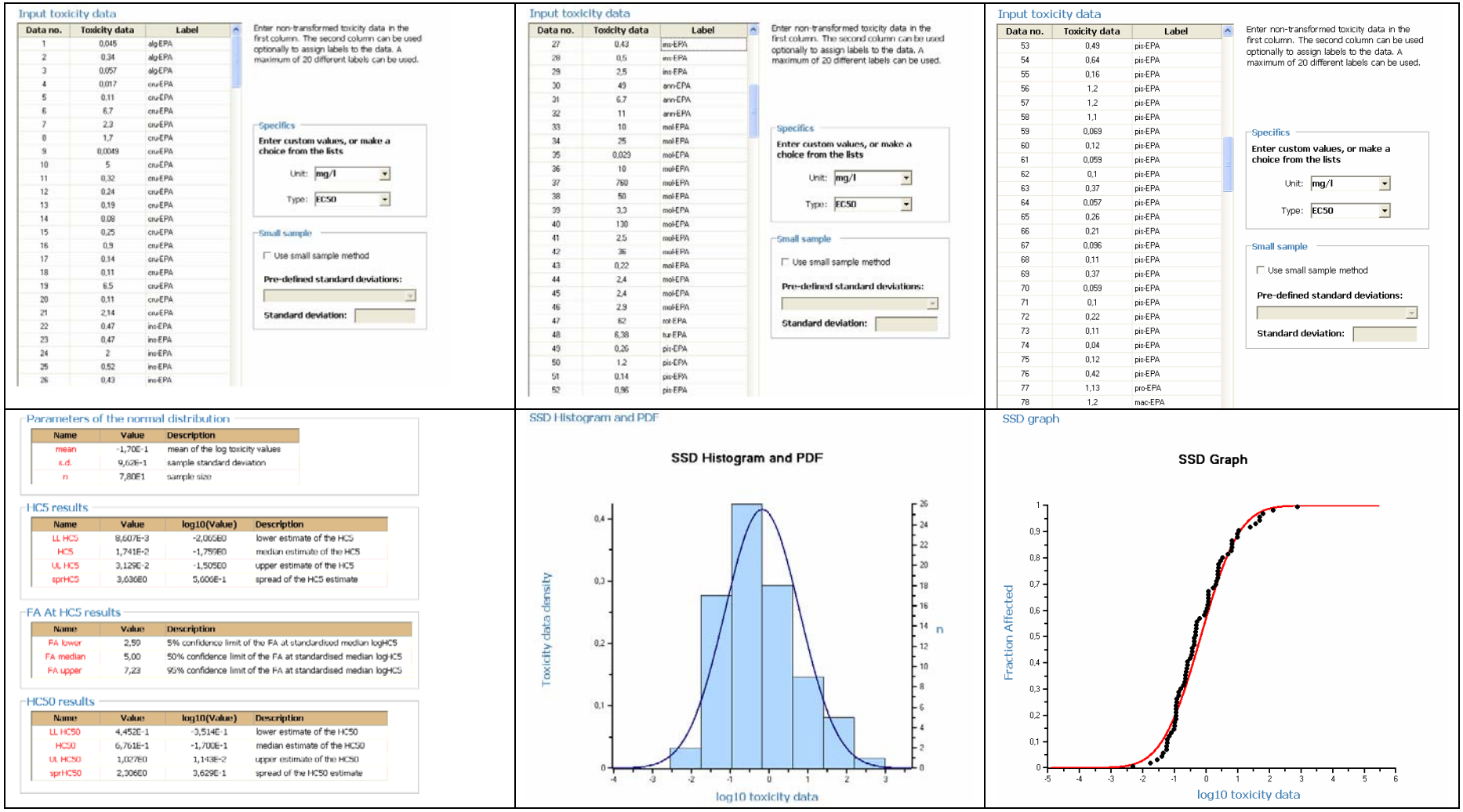
Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Champia parvula (alg)			(14d-MATC)→ extrapolated NOEC=MATC/2	(0.0086)→ 0.0086/2=**0.0043**	EPA	5	M		10		**0.43**
Chlorococcales (alg)	1d-EC50	0.045			EPA	1	F				
Navicula seminulum (alg)	4d-EC50	0.34			EPA	12	F				
Nitzschia closterium (alg)	3d-EC50	0.057			EPA	1	M				
Invertebrates											
Acartia clausi (cru)	4d-LC50	0.017			EPA	1	M				
	4d-LC50	0.11			EPA	1	M				
Americamysis bahia (cru)			(29-51d-MATC) → extrapolated NOEC=MATC/2	(0.043) → 0.043/2 = 0.0215	EPA	3	M				
Artemia salina (cru)	1d-LC50	6.7			EPA	1	M				
Asellus communis (cru)	4d-LC50	2.3			EPA	2	F				
			115d-NOEC	0.051	EPA	3	F				
Asellus intermedius (cru)	4d-LC50	1.7			EPA	1	F				
Cancer irroratus (cru)	4d-LC50	**0.0049**			EPA	2	M	10*		**0.49**	
Carcinus maenas (cru)	2d-LC50	5			EPA	1	M				
Caridina nilotica (cru)	4d-LC50	0.32			EPA	1	F				
Cyclops viridis (cru)	4d-LC50	0.24			EPA	3	F				
Daphnia magna (cru)	4d-LC50	0.19			EPA	6	F				
Daphnia pulex (cru)	2d-LC50	0.08			EPA	7	F				
Diaptomus sp. (cru)	4d-LC50	0.25			EPA	3	F				
Gammarus fasciatus (cru)	4d-LC50	0.90			EPA	1	F				
	4d-LC50	0.14			EPA	4	F				
Gammarus pseudolimnaeus (cru)			98d-NOEC	0.009	EPA	3	F				
Moinodaphnia macleayi (cru)			5d-NOEC	0.0096	EPA	1	F				
Mysidopsis bigelowi (cru)	4d-LC50	0.11			EPA	2	M				
Pandalus montagui (cru)	2d-LC50	6.5			EPA	1	M				

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Penaeus monodon (cru)	4d-LC50	0.11			EPA	1	M				
Streptocephalus proboscideus (cru)	1d-LC50	2.14			EPA	1	F				
Corixa sp. (ins)	4d-LC50	0.47			EPA	3	F				
Dytiscus sp. (ins)	4d-LC50	0.47			EPA	3	F				
Hydropsyche sp. (ins)	2d-LC50	2			EPA	1	F				
Nepa sp. (ins)	4d-LC50	0.52			EPA	3	F				
Pteronarcys dorsata (ins)	4d-EC50	0.43			EPA	2	F				
Ranatra sp. (ins)	4d-LC50	0.43			EPA	3	F				
Stenonema rubrum (ins)	2d-LC50	0.50			EPA	1	F				
Tanytarsus dissimilis (ins)	2d-LC50	2.5			EPA	2	F				
Aeolosoma headleyi (ann)	2d-LC50	49			EPA	5	F				
Dinophilus gyrociliatus (ann)	4d-LC50	6.7			EPA	2	M				
Lumbriculus variegatus (ann)	4d-LC50	11			EPA	1	F				
Anculosa sp. (mol)	2d-LC50	10			EPA	5	F				
Cerastoderma edule (mol)	2d-LC50	25			EPA	1	M				
Chlamys asperrimus (mol)	2d-EC50	0.029			EPA	1	M				
Crepidula fornicata (mol)	4d-LC50	10			EPA	1	M				
Elimia livescens (mol)	2d-LC50	760			EPA	1	F				
Helisoma trivolvis (mol)	4d-LC50	50			EPA	1	F				
Lymnaea emarginata angulata (mol)	2d-LC50	3.3			EPA	1	F				
Lymnaea sp. (mol)	4d-LC50	130			EPA	1	F				
Lymnaea luteola (mol)	4d-LC50	2.5			EPA	3	F				
Mytilus edulis (mol)	4d-LC50	36			EPA	1	M				
Physa heterostropha (mol)	4d-LC50	0.22			EPA	6	F				
Physa integra (mol)	1d-LC50	2.4			EPA	1	F				
Pila globosa (mol)	4d-LC50	2.4			EPA	3	F				
Viviparus bengalensis (mol)	4d-LC50	2.9			EPA	3	F				
Hydra viridissima (cni)			6d-NOEC	0.011	EPA	1	F				
Brachionus calyciflorus (rot)	1d-LC50	62			EPA	1	F				
Dugesia tigrina (tur)	4d-LC50	6.38			EPA	2	F				
Fish											
Carassius auratus (pis)	14d-LC50	0.26			EPA	5	F				
Catla catla (pis)	4d-LC50	1.2			EPA	3	F				

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Cichlasoma bimaculatum (pis)	2d-LC50	0.14			EPA	1	F				
Cirrhinus mrigala (pis)	4d-LC50	0.96			EPA	3	F				
Cyprinodon variegatus (pis)			28d-NOEC	0.029	EPA	1	M				
Danio rerio (pis)	4d-LC50	0.49			EPA	4	F				
Gambusia affinis (pis)	2d-LC50	0.64			EPA	2	F				
Ictalurus punctatus (pis)	26h-LC50	0.16			EPA	4	F				
Labeo bata (pis)	4d-LC50	1.2			EPA	3	F				
Labeo calbasu (pis)	4d-LC50	1.2			EPA	3	F				
Labeo rohita (pis)	4d-LC50	1.1			EPA	3	F				
Lagodon rhomboides (pis)	1d-LC50	0.069			EPA	1	M				
Lepomis macrochirus (pis)	7d-LC50	0.12			EPA	30	F				
Menidia menidia (pis)	4d-LC50	0.059			EPA	2	M				
Micropterus salmoides (pis)	4d-LC50	0.10			EPA	1	F				
Notemigonus crysoleucas (pis)	1d-LC50	0.37			EPA	3	F				
Oncorhynchus mykiss (pis)	4d-LC50	0.057			EPA	29	F				
			20d-NOEC	0.011	EPA	9	F				
Osteichthyes (pis)	9.3h-EC50	0.26			EPA	1	F				
Perca flavescens (pis)	4d-LC50	0.21			EPA	16	F				
Perca fluviatilis (pis)	1d-LC50	0.096			EPA	1	F				
Pimephales promelas (pis)	6d-LC50	0.11			EPA	40	F				
Pleuronectes americanus (pis)	4d-LC50	0.37			EPA	1	M				
Poecilia reticulata (pis)	4d-LC50	0.059			EPA	2	F				
Pomoxis nigromaculatus (pis)	4d-LC50	0.10			EPA	1	F				
Rhinichthys atratulus (pis)	1d-LC50	0.22			EPA	1	F				
Rutilus rutilus (pis)	3d-LC50	0.11			EPA	1	F				
Salmo salar (pis)	1d-LC50	0.040			EPA	3	F				
Salvelinus fontinalis (pis)	4d-LC50	0.12			EPA	32	F				
Tanichthys albonubes (pis)	2d-LC50	0.42			EPA	4	F				
Tilapia mossambica (pis)	4d-LC50	1.13			EPA	3	F				
Other											
Spirostomum ambiguum (pro)	2d-EC50	1.2			EPA	2	F				
Myriophyllum spicatum (mac)			(32d-EC50) → extrapolated NOEC=EC50/3	(21.2) → 21.2/3 = 7.07	EPA	4	F				

*** a factor of 10 was thought sufficient due to the large number of data**

Deriving MAC-QS: 0.0174 mg/L (AF=1; 78 species from 10 major taxonomic groups from 3 trophic levels) → 17.4 µg/L



Deriving AA-QS: 0.00065 mg/L (AF=3; 9 species from 5 taxonomic groups from 3 trophic levels) → 0.22 µg/L
After omitting the outlier for Macrophyta, AA-QS is (0.0037)/3 µg/L = 1.2 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	0,0043	alg-EPA
2	0,0215	cru-EPA
3	0,051	cru-EPA
4	0,009	cru-EPA
5	0,0096	cru-EPA
6	0,011	cni-EPA
7	0,029	pis-EPA
8	0,011	pis-EPA
9	7,07	mac-EPA
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		
25		
26		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-1,56E0	mean of the log toxicity values
s.d.	9,55E-1	sample standard deviation
n	9,00E0	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	3,539E-5	-4,451E0	lower estimate of the HC5
HC5	6,488E-4	-3,188E0	median estimate of the HC5
UL HC5	3,157E-3	-2,501E0	upper estimate of the HC5
sprHC5	8,920E1	1,950E0	spread of the HC5 estimate

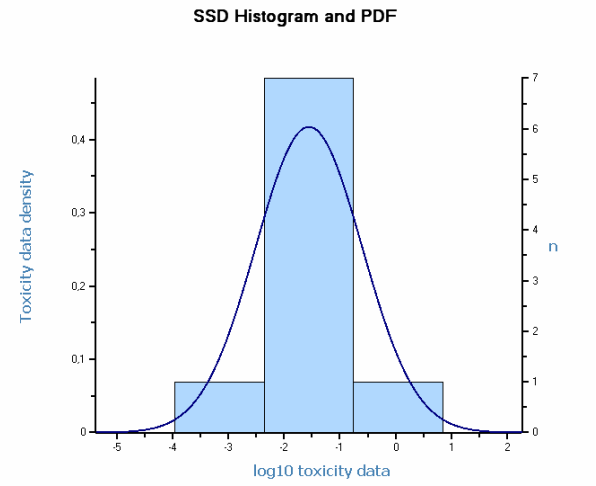
FA At HC5 results

Name	Value	Description
FA lower	0,53	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	21,34	95% confidence limit of the FA at standardised median logHC5

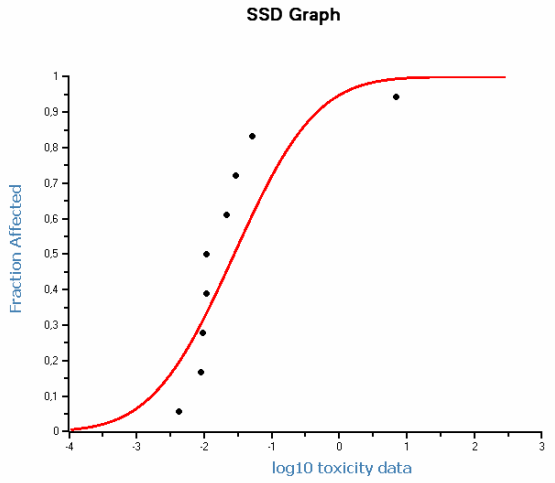
HC50 results

Name	Value	log10(Value)	Description
LL HC50	7,124E-3	-2,147E0	lower estimate of the HC50
HC50	2,786E-2	-1,555E0	median estimate of the HC50
UL HC50	1,089E-1	-9,628E-1	upper estimate of the HC50
sprHC50	1,529E1	1,184E0	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph

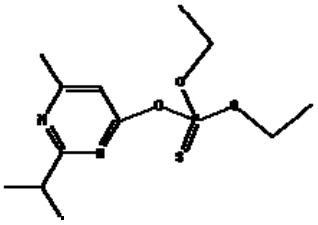


Summary report for Diazinon

SUMMARY

Substance name	**Diazinon**	
CAS-number	**333-41-5**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.0034 µg/L**	**0.034 µg/L**
Sediment	**/**	**/**
Remarks	**data from dossier**	

1. IDENTITY

Substance name	Diazinon
CAS-number	333-41-5
Substance group	Insecticide-Organophosphorus
Synonyms	/
Molecular formula	$C_{12}H_{21}N_2O_3PS$
Structural formula	

Substance name	G 27550*
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

***Metabolite is not relevant due to the low toxicity**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**		**ref.**
Substance	Diazinon	G 27550**	
Molecular weight (g/mol)	304.3	/	dossier
Vapour Pressure (Pa)	1.2E-02	/	dossier
Water Solubility (mg/L)	60	/	dossier
Log Kow	3.69	/	dossier
Log Koc	2.8	0.76	dossier
Log K_{SED}	1.5	-0.55	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	6.1E-02	/	dossier
pKa	2.6	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic			**ref.**
Substance	Diazinon	G 27550	
BCF	**500** (trigger value for subst. with log Kow>3: BCF=100)	/	dossier
(Aerobic bio)degradation	Not readily biodegradable	hydrolytically, photolytically stable	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Diazinon

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	7d-EC50	6.4			PPP dossier	MS	F				
Invertebrates											
	2d-EC50	0.00096			PPP dossier	MS	F				
	(2d-NOEC)	(0.00056)			PPP dossier	MS	F				
Daphnia sp.			21d-NOEC	**0.00017**	PPP dossier	MS	F	5	50	**0.034***	**0.0034**
	2d-EC50	0.00041			PPP dossier	MS	F				
Ceriodaphnia sp.	(2d-NOEC)	(0.00008)			PPP dossier	MS	F				
Fish											
Rainbow trout	4d-LC50	3.1			PPP dossier	MS	F				
	(4d-NOEC)	(0.7)			PPP dossier	MS	F				
Bluegill sunfish	4d-LC50	0.27			PPP dossier	MS	F				
	(4d-NOEC)	(<0.1)			PPP dossier	MS	F				
Fathead minnow			34d-NOEC	0.092	PPP dossier	MS	F				
Other											
Mesocosm test			6m-LOEC	0.0024	PPP dossier	-	F				
			84d-LOEC	0.002	PPP dossier	-	F				
Microcosm test			84d-NOEC	< 0.002	PPP dossier	-	F				

*** MAC-QS derived from NOEC (AF = 1) is protective for Ceriodaphnia sp., which are the most sensitive species**

4.1.2 Aquatic toxicity G 27550

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae						MS	F				
Unknown species	>100										
Daphnids											
Daphnia sp.	2d-EC50	>100									
Fish											
Rainbow trout	4d-LC50	>100				MS	F				
	(4d-NOEC)	(58)				MS	F				

Aquatic toxicity of the metabolite G 27550 is between 10-100 mg/L → metabolite is not relevant due to the low toxicity

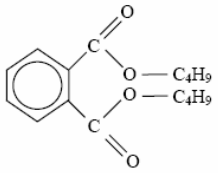
Summary report for Dibutyl Phthalate

SUMMARY

Substance name	**Dibutyl Phthalate**	
CAS-number	**84-74-2**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**10 µg/L**	**100 µg/L**
Sediment	**/**	**/**
Remarks	**EU RAR* data: AA-QS=PNEC (AF = 10) MAC-QS=PNEC*10**	

* EU RISK ASSESSMENT Report, Final Report, DIBUTYL PHTHALATE, Addendum to the Environmental Section, 2004, The Netherlands

1. IDENTITY

Substance name	Dibutyl Phthalate
CAS-number	84-74-2
Substance group	Organics
Synonyms	/
Molecular formula	$C_{16}H_{22}O_4$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	278.34	RAR
Vapour Pressure (Pa)	9.7±3.3E-02	RAR
Water Solubility (mg/L)	10	RAR
Log Kow	4.57	RAR
Log Koc	3.80	RAR
Log K_{SED}	2.50	Est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	0.27	RAR
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	1.8 L/kg (fish)	RAR
(Aerobic bio)degradation	Biodegradable under anaerobic conditions, hydrolytically stable	RAR

Summary report for Dibutyltin compounds

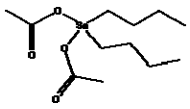
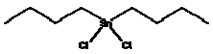
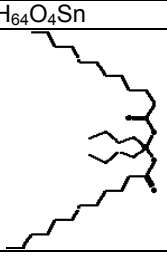
SUMMARY

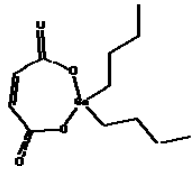
Substance name	**Dibutyltin compounds**	
CAS-number		
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	0.02 nmol/L	0.2 nmol/L
SSD**	**0.09 nmol/L**	**0.9 nmol/L**
Sediment Cas No: 77-58-7	**0.29 mmol/ kg dw**	**2.9 mmol/ kg dw**
Remarks	**Partitioning to sediment is relevant for Dibutyltin dilauraat (Cas No: 77-58-7): AA-QS and MAC-QS is derived for this substance**	

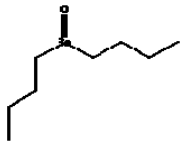
*** marine and freshwater data**

**** AA-QS and MAC-QS derived with SSD are protective**

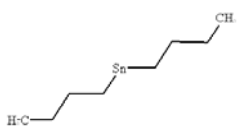
1. IDENTITY

Substance name	Bis(acetyloxy)dibutylstannane
CAS-number	1067-33-0
Substance group	Organics
Synonyms	Dibutyltin diacetate
Molecular formula	$C_{12}H_{24}O_4Sn$
Structural formula	
Substance name	Dibutyldichlorostannane
CAS-number	683-18-1
Substance group	Organics
Synonyms	Dibutyltin dichloride
Molecular formula	$C_8H_{18}Cl_2Sn$
Structural formula	
Substance name	Dibutylbis[(1-oxododecyl)oxy]stannane
CAS-number	77-58-7
Substance group	Organics
Synonyms	Dibutyltin dilauraat
Molecular formula	$C_{32}H_{64}O_4Sn$
Structural formula	

Substance name	2,2-Dibutyl-1,3,2-dioxastannepin-4,7-dione
CAS-number	78-04-6
Substance group	Organics
Synonyms	Dibutyltin maleate
Molecular formula	$C_{12}H_{20}O_4Sn$
Structural formula	

Substance name	Dibutyloxostannane
CAS-number	818-08-6
Substance group	Organics
Synonyms	Dibutyltin oxyde
Molecular formula	$C_8H_{18}OSn$
Structural formula	

Substance name	Dibutyldifluorostannane
CAS-number	563-25-7
Substance group	Organics
Synonyms	/
Molecular formula	$C_8H_{18}F_2Sn$
Structural formula	

Substance name	Dibutyl stannane
CAS-number	1002-53-5
Substance group	Organics
Synonyms	Dibutyltin
Molecular formula	$C_8H_{18}Sn$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property											**ref.**
Substance CAS-number	**1067-33-0**		**683-18-1**		**77-58-7**		**78-04-6**		**818-08-6**		/
Molecular weight (g/mol)	351.01		303.83		631.54		346.98		248.92		http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	0.401	SRC est.	10.5	SRC est.	5.95E-07	SRC est.	3.37E-05	SRC est.	224	SRC est.	SRC
Water Solubility (mg/L)	1233	SRC est.	542.5	SRC est.	8.23E-08	SRC est.	17.4	SRC est.	0.67	SRC est.	SRC
Log Kow	0.81	SRC est.	1.56	SRC exp.	10.64	SRC est.	3.01	SRC est.	5.33	SRC est.	SRC
Log Koc	2.45	SRC	3.35	SRC	7.81	SRC	2.54	SRC	3.18	SRC	SRC
Log K_{SED}	1.15	est. from Koc-5% OC	2.05	est. from Koc-5% OC	6.51	est. from Koc-5% OC	1.24	est. from Koc-5% OC	1.88	est. from Koc-5% OC	/
Henry-coefficient (Pa-m3/mol)	0.114	SRC est.	5.86	SRC est.	4550	SRC est.	0.000672	SRC est.	82600	SRC est.	SRC
pKa											

Property					**ref.**
Substance CAS-number	**563-25-7**		**1002-53-5**		/
Molecular weight (g/mol)	270.92	http://chemfinder.cambridgesoft.com/	232.94	SRC	/
Vapour Pressure (Pa)	0.011	SRC est.	224	SRC est.	SRC
Water Solubility (mg/L)	1503	SRC est.	1567	SRC est.	SRC
Log Kow	1.26	SRC est.	1.49	SRC exp.	SRC
Log Koc	3.35	SRC	2.97	SRC est.	SRC
Log K_{SED}	2.05	est. from Koc-5% OC	1.67	est. from Koc-5% OC	/
Henry-coefficient (Pa-m3/mol)	1970	SRC est.	33.2	SRC est.	SRC
pKa					

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic										
Substance CAS number	**1067-33-0**		**683-18-1**		**77-58-7**		**78-04-6**		**818-08-6**	
BCF	100	SRC est.	3.17	SRC est.	100	SRC est.	1041	SRC est.	6.73E+04	SRC est.
(Aerobic bio)degradation	Not readily biodegradable	SRC	Not readily biodegradable	SRC	Not readily biodegradable	SRC	Not readily biodegradable	SRC	Not readily biodegradable	SRC

Characteristic				
Substance CAS number	**563-25-7**		**1002-53-5**	
BCF	1.88	SRC est.	2.8	SRC est.
(Aerobic bio)degradation	Not readily biodegradable	SRC	Not readily biodegradable	SRC

4. ECOTOXICITY

4.1.1 Aquatic acute and chronic toxicity

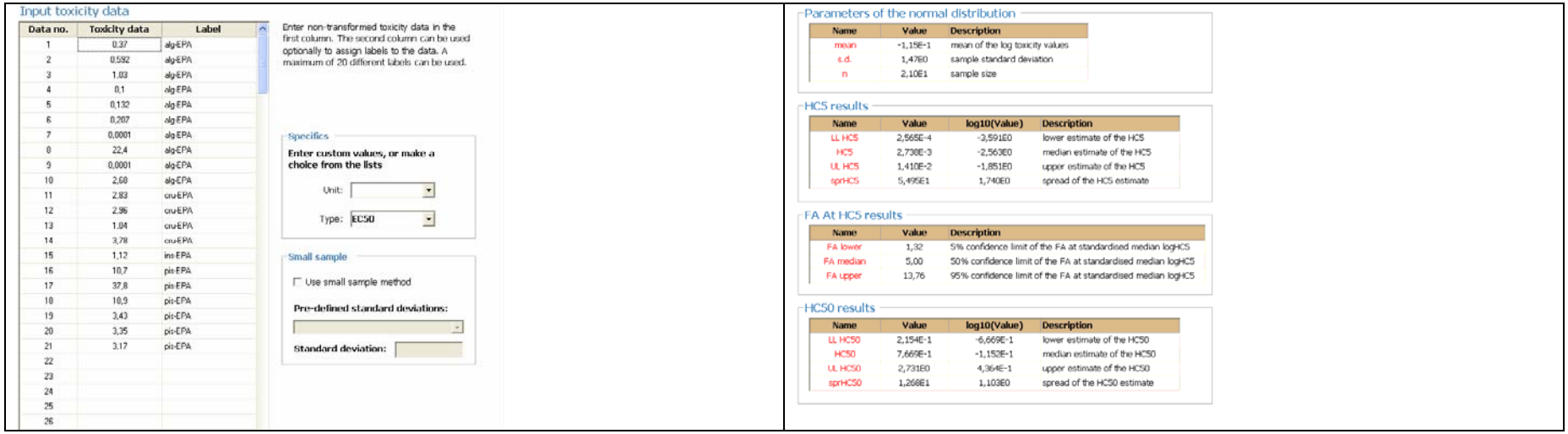
Species	Substance	Endpoint-acute	Value – (µmol/L)	Endpoint-chronic	Value – (µmol/L)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (nmol/L)	AA-QS (nmol/L)
Algae												
Thalassiosira guillardii (alg)	Dibutyltin diacetate	3d-EC50	0.370			EPA	1	M				
	Dibutyltin dichloride	3d-EC50	0.592			EPA	1	M				
	Dibutyldifluorostannane	3d-EC50	1.03			EPA	1	M				
Skeletonema costatum (alg)	Dibutyltin diacetate	3d-EC50	0.10			EPA	3	M				
	Dibutyltin dichloride	3d-EC50	0.132			EPA	3	M				
	Dibutyldifluorostannane	3d-EC50	0.207			EPA	1	M				
Platymonas sp. (alg)	Dibutyltin dichloride	4d-EC50	**0.0001**			EPA	1	M				
Ankistrodesmus falcatus acicul (alg)	Dibutyltin dichloride	4h-EC50	22.4			EPA	1	F				
Scenedesmus acutus (alg)	Dibutyltin dichloride	4d-EC50	0.0001			EPA	2	F				
Scenedesmus subspicatus (alg)	Dibutyltin lauraat			4d-EC10*	1.58	EPA	2	F				
	Dibutyltin oxyde			3d-EC10*	0.96	EPA	2	F				
		3d-EC50	2.69			EPA	2	F				
Invertebrates												
Rhithropanopeus harrisii (cru)	Dibutyltin dichloride	14d-LC50	2.83			EPA	1	M				
Daphnia magna (cru)	Dibutyltin dichloride	1d-EC50	2.96			EPA	1	F				
	Dibutyltin lauraat	1d-EC50	1.04			EPA	1	F				
	Dibutyltin oxyde	1d-EC50	3.78			EPA	1	F				
Culex pipiens (ins)	Dibutyltin lauraat	1d-LC50	1.12			EPA	1	F				
Mytilus edulis (mol)	Dibutyl stannane			33d-NOEC	0.009	EPA	1	M				
Fish												
Oryzias latipes (pis)	Dibutyltin diacetate	2d-LC50	10.7			EPA	1	F				
	Dibutyltin maleate	2d-LC50	37.8			EPA	1	F				
	Dibutyltin dichloride	2d-LC50	18.9			EPA	1	F				
				28d-NOEC	1050	EPA	1	F				
	Dibutyltin lauraat	2d-LC50	3.43			EPA	1	F				
	Dibutyltin oxyde	2d-LC50	3.35			EPA	1	F				
Oncorhynchus mykiss (pis)	Dibutyltin dichloride			(110d-LOEC)* → LOEC/2 = NOEC	**0.00046/2 = 0.00023**	EPA	2	F	1	10	**0.23**	**0.023**
Poecilia reticulate (pis)	Dibutyltin dichloride			1m-NOEC	7.73	EPA	2	F				
Leuciscus idus (pis)	Dibutyltin lauraat	2d-LC50	3.17			EPA	1	F				

*** additional data**

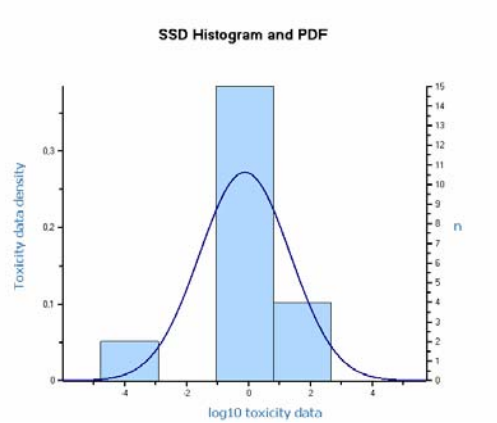
4.2 Sediment toxicity

Equilibrium partitioning (EP) method-calculated for Dibutyltin dilauraat (Cas No: 77-58-7) with log Ksed = 6.51
AA-QS sed = 3235937 L/kg*0.09 nmol/L = 0.29 mmol/ kg dw
MAC-QS sed = 3235937 L/kg*0.9 nmol/L = 2.9 mmol/kg dw

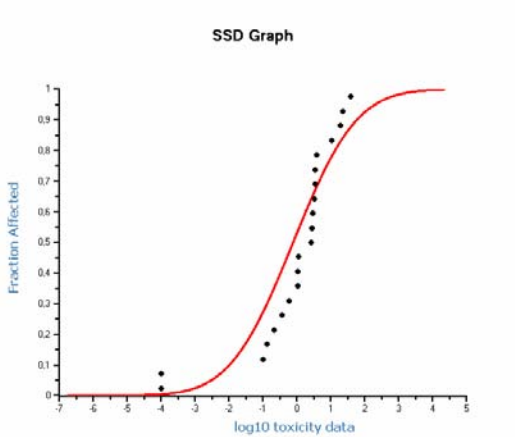
Deriving MAQ-QS: 0.00274 µmol/L (AF=3; 21 species from 4 major taxonomic groups from 3 trophic levels) → 0.91 nmol/L
Deriving AA-QS: 0.91/10 = 0.091 nmol/L



SSD Histogram and PDF



SSD graph



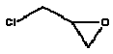
Summary report for Epichlorhydrin

SUMMARY

Substance name	**Epichlorhydrin**	
CAS-number	**106-89-8**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	**12 µg/L**	**120 µg/L**
Sediment	**/**	**/**
Remarks	**/**	**/**

*** marine and freshwater data**

1. IDENTITY

Substance name	Epichlorhydrin
CAS-number	106-89-8
Substance group	Organic
Synonyms	/
Molecular formula	C_3H_5ClO
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	92.5249	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	2.19E+03	SRC exp.
Water Solubility (mg/L)	65900	SRC exp.
Log Kow	0.5	SRC exp.
Log Koc	0.6	SRC est.
Log K_{SED}	-0.6	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	3.1	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	3	SRC est.
(Aerobic bio)degradation	Readily biodegradable	HSDB

4. ECOTOXICITY

4.1.2 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Scenedesmus quadricauda (alg)			8d-NOEC	2.7	IUCLID	1	F				
Invertebrates											
Daphnia magna (cru)	2d-LC50	23.9			RIVM database	3	F				
Daphnia sp. (cru)	1d-EC50	34.6			IUCLID	>2	F				
Fish											
Carassius auratus (pis)	1d-LC50	23			RIVM database	1	F				
Danio rerio (pis)	4d-LC50	31			RIVM database	1	F				
Lepomis macrochirus (pis)	4d-LC50	35			RIVM database	1	F				
Leuciscus idus melanotus (pis)	2d-LC50	24			RIVM database	1	F				
Pimephales promelas (pis)	4d-LC50	12.1			RIVM database	3	F				
Rasbora heteromorpha (pis)	2d-LC50	36			RIVM database	1	F				
Menidia beryllina (pis)	4d-LC50	18			RIVM database	1	M				
Cyprinodon variegatus (pis)	4d-LC50	**11.8**			IUCLID	1	M	100	1000	**118**	**11.8**
Other											
Pseudomonas putida (bac)			16h-NOEC	28	IUCLID	1	F				

Summary report for Fluorides

SUMMARY

Substance name	**Fluorides**	
CAS-number	**16984-48-8**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	0.19 mg/L	1.1 mg/L
SSD	**0.68 mg/L**	**6.8 mg/L**
Sediment	**/**	**/**
Remarks	MPC=1.5 mg/L **	**/**

*** marine and freshwater data**

**** Sloof, W., Eerens, H.C., Janus, J.A., Pos, J.P.M., Integrated criteria document fluorides, Rivm, Bilthoven, The Netherlands, 1989**

1. IDENTITY

Substance name	Fluorides
CAS-number	16984-48-8
Substance group	Inorganics
Synonyms	/
Molecular formula	F^-
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	18.9984	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log Kow	/	
Log Koc	/	
Log K_{SED}	/	
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	Ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (mg/l)	AA-QS (mg/l)
Algae											
Chlorella vulgaris (alg)	3d-LC50	133	3d-NOEC	**9.5**	EPA	2	F		50		**0.19**
Scenedesmus subspicatus (alg)	3d-EC50	850			EPA	3	F				
Skeletonema costatum (alg)	4d-EC50	181			EPA	1	M				
Invertebrates											
Ceratopsyche bronta (ins)	6d-EC50	**11.5**			EPA	1	F	10		**1.1**	
Cheumatopsyche pettiti (ins)	6d-EC50	24				1	F				
Chimarra marginata (ins)	4d-EC50	36			EPA	3	F				
Hydropsyche bulbifera (ins)	4d-EC50	21			EPA	3	F				
Hydropsyche exocellata (ins)	4d-EC50	23			EPA	3	F				
Hydropsyche lobata (ins)	4d-EC50	39			EPA	3	F				
Hydropsyche occidentalis (ins)	6d-EC50	24			EPA	1	F				
Hydropsyche pellucidulla (ins)	4d-EC50	27			EPA	3	F				
Streptocephalus proboscideus (cru)	1d-LC50	70			EPA	1	F				
Ceriodaphnia dubia (cru)	1d-LC50	158			EPA	1	F				
Ceriodaphnia pulchella (cru)	1d-LC50	83			EPA	1	F				
Daphnia carinata (cru)	1d-LC50	354			EPA	1	F				
			14d-LOEC*	50	EPA	1	F				
Daphnia magna (cru)	2d-LC50	219			EPA	14	F				
			21d-NOEC	14	EPA	2	F				
			14d-LOEC*	50	EPA	1	F				
Daphnia pulex (cru)	1d-EC50	221			EPA	1	F				
Simocephalus vetulus (cru)	1d-EC50	202			EPA	1	F				
Artemia salina (cru)	1d-LC50	3040			EPA	1	M				
Crangon crangon (cru)	2d-LC50	300			EPA	1	M				
Penaeus indicus (cru)	4d-LC50	1118			EPA	1	M				
Americamysis bahia (cru)	4d-LC50	23			EPA	1	M				
Crassostrea gigas (mol)	2d-EC50	58			EPA	2	M				
Fish											

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	Ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (mg/l)	AA-QS (mg/l)
Lepomis macrochirus (pis)	4d -LC50	830			EPA	1	F				
Salmo trutta fario (pis)	8d- LC50	98			EPA	2	F				
Pimephales promelas (pis)	4d- LC50	246			EPA	4	F				
Oncorhynchus mykiss (pis)	4d -LC50	64			EPA	8	F				
Gambusia affinis (pis)	4d -LC50	418			EPA	1	F				
Gasterosteus aculeatus (pis)	4d -LC50	390			EPA	3	F				
Cyprinodon variegates (pis)	4d -LC50	500			EPA	1	M				
Other											
Brachionus calyciflorus (rot)	1d- LC50	183			EPA	1	F				
Philodina acuticornis (rot)	1d- EC50	158			EPA	1	F				

*** Additional data**

Deriving MAC-QS: 13.5 mg/L (AF=2; 32 species from 6 major taxonomic groups from 3 trophic levels) → 6.8 mg/L
Deriving AA-QS: 6.8/10 = 0.68 mg/L

Input toxicity data

Data no.	Toxicity data	Label
1	133	alg-EPA
2	950	alg-EPA
3	181	alg-EPA
4	11,5	ins-EPA
5	24	ins-EPA
6	36	ins-EPA
7	21	ins-EPA
8	23	ins-EPA
9	39	ins-EPA
10	24	ins-EPA
11	27	ins-EPA
12	70	cru-EPA
13	158	cru-EPA
14	83	cru-EPA
15	354	cru-EPA
16	219	cru-EPA
17	221	cru-EPA
18	202	cru-EPA
19	3040	cru-EPA
20	300	cru-EPA
21	1118	cru-EPA
22	23,3	cru-EPA
23	58	mol-EPA
24	930	pis-EPA
25	98	pis-EPA
26	246	pis-EPA

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Input toxicity data

Data no.	Toxicity data	Label
27	64	pis-EPA
28	418	pis-EPA
29	390	pis-EPA
30	500	pis-EPA
31	183	rot-EPA
32	158	rot-EPA
33		
34		
35		
36		
37		
38		
39		
40		
41		
42		
43		
44		
45		
46		
47		
48		
49		
50		
51		
52		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	2,11E0	mean of the log toxicity values
s.d.	5,91E-1	sample standard deviation
n	3,20E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	6,493E0	8,125E-1	lower estimate of the HC5
HC5	1,346E1	1,129E0	median estimate of the HC5
UL HC5	2,319E1	1,365E0	upper estimate of the HC5
sprHC5	3,571E0	5,528E-1	spread of the HC5 estimate

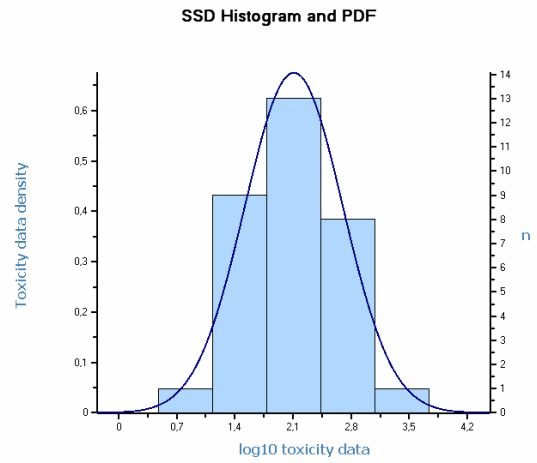
FA At HC5 results

Name	Value	Description
FA lower	1,76	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	9,66	95% confidence limit of the FA at standardised median logHC5

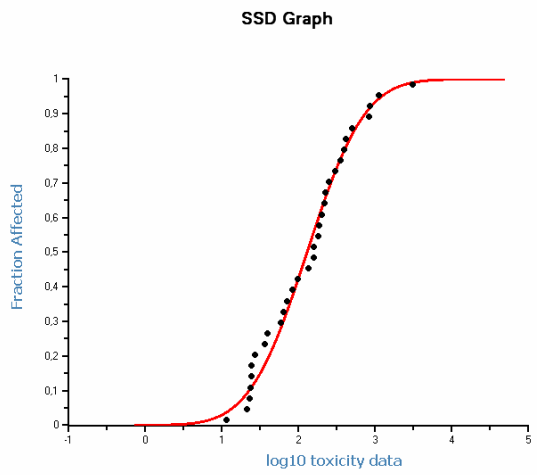
HC50 results

Name	Value	log10(Value)	Description
LL HC50	8,567E1	1,933E0	lower estimate of the HC50
HC50	1,288E2	2,110E0	median estimate of the HC50
UL HC50	1,936E2	2,287E0	upper estimate of the HC50
sprHC50	2,260E0	3,540E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



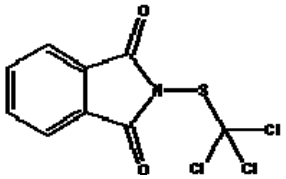
Summary report for Folpet

SUMMARY

Substance name	**Folpet**	
CAS-number	**133-07-3**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.098 µg/L***	**0.98 µg/L***
Sediment	**/**	**/**
Remarks	**data from dossier**	

*** Due to rapid degradation it is unlikely for the Folpet to occur in water**

1. IDENTITY

Substance name	Folpet
CAS-number	133-07-3
Substance group	Fungicide-Thiophthalimide
Synonyms	/
Molecular formula	$C_9H_4Cl_3NO_2S$
Structural formula	

Substance name	Phthalimide*
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	Phthalamic acid*
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	Phthalic acid*
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

***Metabolite is not relevant due to the low toxicity**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**				**ref.**
Substance	Folpet	Phthalimide	Phthalamic acid	Phthalic acid	
Molecular weight (g/mol)	296.6	/	/	/	dossier
Vapour Pressure (Pa)	2.1E-05	/	/	/	dossier
Water Solubility (mg/L)	0.80	/	/	/	dossier
Log Kow	3.017 (at 20 ^{0}C)	/			dossier
Log Koc	not measurable due to rapid hydrolysis	2.32	1.86	1.0	dossier
Log K_{SED}	/	1.02	0.56	-0.30	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	8.0E-03	/	/	/	dossier
pKa	No	/	/	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic					**ref.**
Substance	Folpet	Phthalimide	Phthalamic acid	Phthalic acid	
BCF	56 (trigger value for readily degradable compound: 1000)	/	/	/	dossier
(Aerobic bio) degradation	Rapid hydrolytic degradation (days), Inherently/Readily degradable	/	/	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Folpet

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Scenedesmus subspicatus	3d-EC50	>10			PPP dossier	MS	F				
Daphnids											
/											
Fish											
Rainbow trout	4d-LC50	0.233			PPP dossier	MS	F				
Brown trout	4d-LC50	**0.098**			PPP dossier	MS	F	100	1000	**0.98**	**0.098**

4.1.2 Aquatic toxicity Phtalimide

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
/											
Daphnids											
Daphnia magna	2d-EC50	39			PPP dossier	MS	F				
Fish											
Bluegill sunfish	4d-LC50	38			PPP dossier	MS	F				

Aquatic toxicity of the metabolite Phtalimide is between 10-100 mg/L → metabolite is not relevant due to the low toxicity

4.1.3 Aquatic toxicity Phtalamic acid

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornotum	3d-EC50	>100				MS	F				
Daphnids											
Daphnia magna	2d-EC50	≥100				MS	F				
Fish											
Rainbow trout	4d-LC50	>100				MS	F				

Aquatic toxicity of the metabolite Phtalamic acid is >100 mg/L → metabolite is not relevant due to the low toxicity

4.1.4 Aquatic toxicity Phtalic acid

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornotum	3d-EC50	>100				MS	F				
Daphnids											
Daphnia magna	2d-EC50	≥100				MS	F				
Fish											
Rainbow trout	4d-LC50	>100				MS	F				

Aquatic toxicity of the metabolite Phtalic acid is >100 mg/L → metabolite is not relevant due to the low toxicity