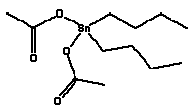
Summary report for Dibutyltin compounds

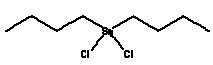
SUMMARY

Substance name	**Dibutyltin compounds**	
CAS-number		
Proposed	**Freshwater***	
Quality Standard	**AA-QS**	**MAC-QS**
Water AF **SSD****	0.02 nmol/L = 0.005 µg/L **0.09 nmol/L = 0.02 µg/L****	0.2 nmol/L = 0,05 µg/L **0.9 nmol/L = 0.21 µg/L****
Sediment **Cas No: 77-58-7**	**0.29 mmol/kg dw=68 mg/kg*****	**2.9 mmol/ kg dw= 680 mg/kg*****
Remarks	**Partitioning to sediment is relevant for Dibutyltin dilauraat (Cas No: 77-58-7): AA-QS and MAC-QS is derived for this substance**	

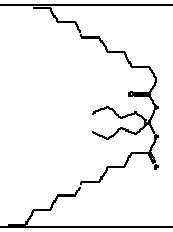
*** marine and freshwater data**
**** AA-QS and MAC-QS derived with SSD are protective**
***** µg/L $C_8H_{18}Sn$**
***** mg/kg $C_8H_{18}Sn$**

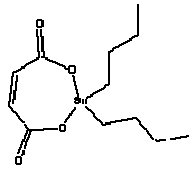
1. IDENTITY

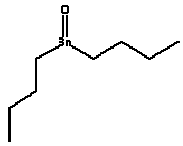
Substance name	Bis(acetyloxy)dibutylstannane
CAS-number	1067-33-0
Substance group	Organics
Synonyms	Dibutyltin diacetate
Molecular formula	$C_{12}H_{24}O_4Sn$
Structural formula	

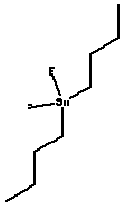
Substance name	Dibutyldichlorostannane
CAS-number	683-18-1
Substance group	Organics
Synonyms	Dibutyltin dichloride
Molecular formula	$C_8H_{18}Cl_2Sn$
Structural formula	

Substance name	Dibutylbis[(1-oxododecyl)oxy]stannane
CAS-number	77-58-7
Substance group	Organics
Synonyms	Dibutyltin dilauraat
Molecular formula	$C_{32}H_{64}O_4Sn$

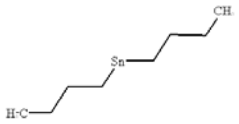
Structural formula	

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

Input toxicity data

Data no.	Toxicity data	Label
1	0,37	alg-EPA
2	0,592	alg-EPA
3	1,03	alg-EPA
4	0,1	alg-EPA
5	0,132	alg-EPA
6	0,207	alg-EPA
7	0,0001	alg-EPA
8	22,4	alg-EPA
9	0,0001	alg-EPA
10	2,68	alg-EPA
11	2,83	cru-EPA
12	2,96	cru-EPA
13	1,04	cru-EPA
14	3,78	cru-EPA
15	1,12	ins-EPA
16	10,7	pis-EPA
17	37,8	pis-EPA
18	10,9	pis-EPA
19	3,43	pis-EPA
20	3,35	pis-EPA
21	3,17	pis-EPA
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:

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-1,15E-1	mean of the log toxicity values
s.d.	1,47E0	sample standard deviation
n	2,10E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	2,565E-4	-3,591E0	lower estimate of the HC5
HC5	2,738E-3	-2,563E0	median estimate of the HC5
UL HC5	1,410E-2	-1,851E0	upper estimate of the HC5
sprHC5	5,495E1	1,740E0	spread of the HC5 estimate

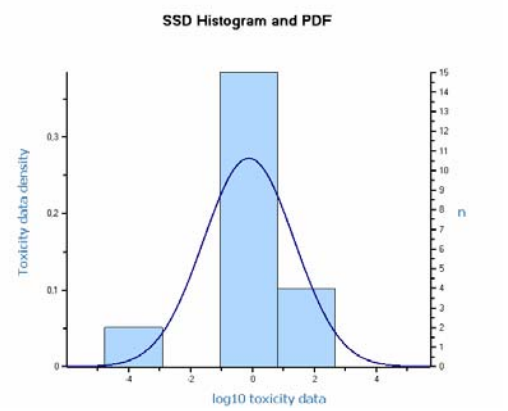
FA At HC5 results

Name	Value	Description
FA lower	1,32	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	13,76	95% confidence limit of the FA at standardised median logHC5

HC50 results

Name	Value	log10(Value)	Description
LL HC50	2,154E-1	-6,669E-1	lower estimate of the HC50
HC50	7,669E-1	-1,152E-1	median estimate of the HC50
UL HC50	2,731E0	4,364E-1	upper estimate of the HC50
sprHC50	1,268E1	1,103E0	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph