

Environmental Hazard & Risk Assessment

CASE STUDY

Tasks:

1. Classify chemical substances (caprolactame, diphenylamine, dioctylphthalate) for environmental hazard
2. Define endangered environmental compartments based on P-CH properties
3. Perform effects assessment – calculate Predicted No Effect Concentration (**PNEC**)

Environmental Hazard / Risk Assessment – Case Study

Results

Caprolactame		
Classification	GHS Pictogram	
Effects assessment		
	PNEC	
Proposals / comments:		

Diphenylamine		
Classification	GHS Pictogram	
Effects assessment		
	PNEC	
Proposals / comments:		

Bis (2-ethylhexyl)phthalate (DEHP)		
Classification	GHS Pictogram	
Effects assessment		
	PNEC	
Proposals / comments:		

Tables

Estimates for the emission factors (fractions released)

Conditions Solubility (mg/l)	Vap. (Pa)	Emission factors to:		
		Air	Waste water	Soil
<100	< 100	0.65	0.25	0.0005
	100 – 1 000	0.8	0.1	0.0025
	≥ 1 000	0.95	0.05	0.001
100 – 1000	< 100	0.4	0.5	0.005
	100 – 1 000	0.55	0.35	0.002
	≥ 1 000	0.65	0.25	0.001
1 000 - 10 000	< 100	0.25	0.65	0.005
	100 – 1 000	0.35	0.55	0.002
	≥ 1 000	0.5	0.4	0.001
≥ 10 000	< 100	0.05	0.85	0.005
	100 – 1 000	0.1	0.8	0.002
	≥ 1 000	0.25	0.65	0.001

Overall emissions concerning production volume:

< 1000 per annum – 0,02

> 1000 per annum – 0,002 – 0,0005

Classes of affinity of chemicals for the different environmental compartments in relation to the physico-chemical characteristics of the molecules

Affinity	WATER	AIR	SOIL	ANIMAL BIOTA	PLANT BIOTA
	S v mg/l	H v Pa m ³ /mol	log Koc	log Kow	log Koa
high	> 10 000	> 10	> 5	> 5	> 8
medium high	10 000 – 100	10 – 10 ⁻¹	5 – 4	5 – 3.5	8 – 7
medium	100 – 10	10 ⁻¹ – 10 ⁻²	4 – 2	3.5 – 3	7 – 5
medium low	10 – 0,1	10 ⁻² – 10 ⁻⁴	2 – 1	3 – 1	> 4
low	< 0,1	< 10 ⁻⁴	< 1	< 1	< 4

S = water solubility

H = Henry law constant

Koc = Soil Adsorptive Coefficient

Kow = octanol/water distribution coefficient

Koa = oktanol/air distribution coefficient

Units recalculation

1 atm = 1013 mbar = 1013 hPa = 101300 Pa = 760 mmHg

1 mmHg = 133,3 Pa

Classification categories for hazardous to the aquatic environment

REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008

Acute (short-term) aquatic hazard

Acute Category 1 (Note 1)

96 hr LC₅₀ (for fish) \leq 1 mg/l and/or

48 hr EC₅₀ (for crustacea) \leq 1 mg/l and/or

72 or 96 hr ErC₅₀ (for algae or other aquatic plants) \leq 1 mg/l. (Note 2)

Chronic (long-term) aquatic hazard

Chronic Category 1 (Note 1)

96 hr LC₅₀ (for fish) \leq 1 mg/l and/or

48 hr EC₅₀ (for crustacea) \leq 1 mg/l and/or

72 or 96 hr ErC₅₀ (for algae or other aquatic plants) \leq 1 mg/l (Note 2)

and the substance is not rapidly degradable and/or the experimentally determined BCF \geq 500 (or, if absent, the log K_{ow} \geq 4).

Chronic Category 2

96 hr LC₅₀ (for fish) > 1 to \leq 10 mg/l and/or

48 hr EC₅₀ (for crustacea) > 1 to \leq 10 mg/l and/or

72 or 96 hr ErC₅₀ (for algae or other aquatic plants) > 1 to \leq 10 mg/l (Note 2)

and the substance is not rapidly degradable and/or the experimentally determined BCF \geq 500 (or, if absent, the log K_{ow} \geq 4), unless the chronic toxicity NOECs are > 1 mg/l.

Chronic Category 3

96 hr LC₅₀ (for fish) > 10 to \leq 100 mg/l and/or

48 hr EC₅₀ (for crustacea) > 10 to \leq 100 mg/l and/or

72 or 96 hr ErC₅₀ (for algae or other aquatic plants) > 10 to \leq 100 mg/l (Note 2)

and the substance is not rapidly degradable and/or the experimentally determined BCF \geq 500 (or, if absent, the log K_{ow} \geq 4) unless the chronic toxicity NOECs are > 1 mg/l.

Chronic Category 4

Cases when data do not allow classification under the above criteria but there are nevertheless some grounds for concern. This includes, for example, poorly soluble substances for which no acute toxicity is recorded at levels up to the water solubility (note 3), and which are not rapidly degradable and have an experimentally determined BCF \geq 500 (or, if absent, a log K_{ow} \geq 4), indicating a potential to bioaccumulate, will be classified in this category unless other scientific evidence exists showing classification to be unnecessary. Such evidence includes chronic toxicity NOECs $>$ water solubility or > 1 mg/l, or evidence of rapid degradation in the environment.

Note 1

When classifying substances as Acute Category 1 and/or Chronic Category 1 it is necessary at the same time to indicate an appropriate M-factor (see table 4.1.3).

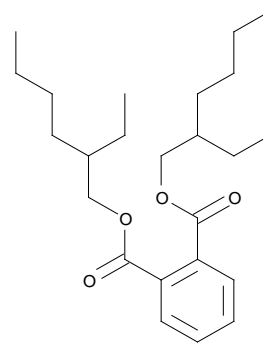
Note 2

Classification shall be based on the ErC₅₀ [= EC₅₀ (growth rate)]. In circumstances where the basis of the EC₅₀ is not specified or no ErC₅₀ is recorded, classification shall be based on the lowest EC₅₀ available.

Note 3

'No acute toxicity' is taken to mean that the L(E)C₅₀(s) is/are above the water solubility. Also for poorly soluble substances, (water solubility < 1 mg/l), where there is evidence that the acute test does not provide a true measure of the intrinsic toxicity.

DIOCTYLPHTHALATE



1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester

CAS No.:	117-81-7
EINECS/ELINCS No.:	204-211-0
RTECS No.:	TI0350000

1. Hazard properties

1.1 EU Classification

Index. No.:

Classification:	
Risk phrases:	
Safety phrases:	

Name:	Bis (2-ethylhexyl)phthalate (DEHP)
CAS No.:	117-81-7
Formula:	C24-H38-O4
Molecular weight:	390,54 g/mol
Form:	light colored liquid; colorless oily liquid; slight odor

Melting point:	-50°C	Boiling point:	230 °C pri 5mm Hg
Flash point:	215 °C (open cup)		[R 13]
Autoignition temperature:	390 °C		[R 13]
Vapor pressure:	1,32 mm Hg pri 200 °C; 9,75x10 ⁻⁶ mm Hg pri 25 °C		[HSDB]
Henry constant:	1,1x10 ⁻⁵ atm x m ³ /mol; log H (Pa.m ³ .mol ⁻³) = -2,8		
Density:	0,9861 at 20 °C		[HSDB]
Water solubility:	less then 0,01% at 25 °C		[HSDB]
	0,340 mg/l at 25 °C		[HSDB]
Solubility in organic solvents:	miscible with mineral oil and hexane		
Log Kow:	7,60 [EPIWinv.2,0]	BCF:	640 [IUCL104]
Ready biodegradability:	No		
Inherent biodegradability:	Yes		
Soil Adsorptive Coefficient	Koc = 165400; logKoc = 5,219 [EPIWin v.2.0]		
Half-life of deg.	7 days (model. river), 60 days (model. lake)		
Photolysis			
Hydrolysis	half-live: at pH 8 = 195 days; at pH 7 = 5 years		

2. Production and use

2.1 Production and use categories

Type	Categories
type	wide dispersive use
industry	Basic chemical industry: basic chemicals Chemical industry: use in synthesis
use	Lubricants and additives
use	Fotochemicals, Solvents, Stabilisators, Vulcanizing agent

Ecotoxicology

Microorganisms

Taxonomic group	Sp.	Effect	Parameter	Effective conc.	Units	Test duration	Lit.
Bacteria	<i>Pseudomonas putida</i>		EC10	>1400	mg/l	6 h	[IUC141]
	<i>Fauschlam</i>		EC0	100	mg/l	30 d	[IUC142]

Water organisms

Short-term studies

Taxon. group	Sp.	Effect	Parameter	Effective conc.	Units	Test duration	Lit.
Fish	<i>Gasterosteus aculeatus</i>	NOEC LC0 LC50 EC50	> = 0,3 > = 0,3 > 0,3 > 0,3	mg/l mg/l mg/l mg/l		96 h 96 h 96 h 96 h	[IUC126]
	<i>Jordanella floridae</i>	NOEC LC50	> = 0,32 > 0,32	mg/l mg/l		96 h 96 h	[IUC126]
	<i>Leuciscus idus</i>	LC0 LC50	22 61	mg/l mg/l		48 h 48 h	[IUC124]
	<i>Leuciscus idus</i>	LC0 LC50	11 533	mg/l mg/l		48 h 48 h	[IUC124]
	<i>Leuciscus idus</i>	NOEC LC50	10 000 > 10 000	mg/l mg/l		96 h 96 h	[IUC127]
Crustaceans	<i>Daphnia magna</i>	LC50	> 0,32	mg/l		48 h	[IUC86]
	<i>Daphnia magna</i>	LC50 LC50	11 > 64	mg/l mg/l		48 h 24 h	[IUC128]
	<i>Daphnia magna</i>	LC50	9,4	mg/l		48 h	[IUC129]
	<i>Daphniapulex</i>	LC50	> 0,4	mg/l		96 h	[IUC131]
Algae	<i>Selenastrum capricornutum</i>	EC50	> 0,1	mg/l		96 h	[IUC132]
	<i>Gymnodinium breve</i>	LC50	100	g/l		96 h	[IUC139]
	<i>Gymnodinium breve</i>	EC50 LC50	31 100	g/l g/l		96 h 96 h	[IUC139]

Terrestrial organisms

Toxicity – soil organisms

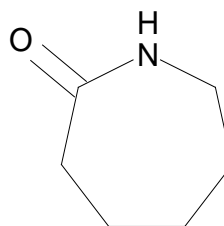
Sp.	Effect	Parameter	Eff. conc.	Units	Test duration	Lit.
<i>Eisenia fetida</i>		mort.	>25	mg/cm ² filt. pap.	48 h	[IUC149]

Toxicity - terrestrial plants

Sp.	Effect	Parameter	Eff. conc.	Units	Test duration	Lit.
<i>Pisum sativum</i>		EC0	> 1000	mg/l		[IUC150]
<i>Sojabohne</i>		EC0	> 390	mg/l	5 d	

Ecotoxicological properties

Caprolactame

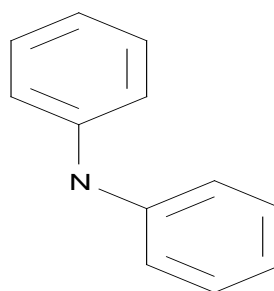


2H-Azepin-2-one, hexahydro-

Substance	Caprolactame
CAS No.	105-60-2
EC No.	203-313-2
Formula	C ₆ H ₁₁ ON
Molecular weight [g/mol]	113.16
Relative density [g/cm ³]	1.014
Melting point [°C]	69 – 71
Boiling point [°C]	270
Water solubility [mg/l]	820000 2000
Vapore pressure [mm Hg]	0.001
Henryho constant [atm×m ³ /mol]	evaporation not significant
log K _{ow}	- 0.19
Hydrolysis, t _{1/2} [days]	n.a.
Photolysis, t _{1/2} [days]	n.a.
Ready biodegradability [%]	82 (MITI I test) 95 – 100 (14 days)
Bioaccumulation, BCF	< 1
Toxicity, microorganisms [mg/l]	EC10 = 1740 (<i>Pseudomonas</i>) EC50 = 4200 (<i>Pseudomonas</i>)
Toxicity, algae [mg/l]	EC50 = 130 (<i>Scenedesmus subspicatus</i>)
Toxicity, crustations [mg/l]	EC50 > 500 (<i>Daphnia magna</i>)
Toxicity, fish [mg/l]	LC50 = 930 (<i>Lepomis macrochirus</i>) Toxicity = 5000 – 10000 NOEC = 1000
Soil Adsorptive Coefficient	Koc = 57,35; logKoc = 1,759

Ecotoxicological properties

Diphenylamine



Benzenamine, N-phenyl-

Substance	Diphenylamine
CAS No.	122-39-4
EC No.	204-539-4
Formula	C ₁₂ H ₁₁ N
Molecular weight [g/mol]	169.22
Relative density [g/cm ³]	
Melting point [°C]	53 – 54
Boiling point [°C]	302
Water solubility [mg/l]	200 - 300 40
Vapore pressure [mm Hg]	1.61×10 ⁻⁴ (20°C) 0.11
Henryho constant [atm×m ³ /mol]	0.90×10 ⁻⁶
log K _{ow}	3.5 3.62
Hydrolysis, t _{1/2} [days]	
Photolysis, t _{1/2} [days]	0.08 – 1.4 (reaction product: karbazol)
Ready biodegradability [%]	0 (MITI I)
Bioaccumulation, BCF	51 – 253 (<i>Cyprinus carpio</i>) 30 (<i>Pimephales promelas</i>) 70
Toxicity, microorganisms [mg/l]	Inhibition > 10 (saprophytic microflora) NOEC = 100 (<i>Nitrosomonas sp.</i>) NOEC = 1000 (<i>Pseudomonas fluorescens</i>)
Toxicity, algae [mg/l]	EC50 = 0.048 (<i>Scenedesmus</i>)
Toxicity, crustations [mg/l]	EC50 = 2.3 (<i>Daphnia magna</i>) EC0(21 days) = 0.16 (<i>Daphnia magna</i>) EC70(21 days) = 0.5 (<i>Daphnia magna</i>)
Toxicity, fish [mg/l]	LC50 = 1 – 100 LC50(48 h) = 5.1 (<i>Oryzias latipes</i>)
Toxicity, earthworms [mg/kg]	LC50(14 days) = 269 NOEC(14 days) = 178
Soil Adsorptive Coefficient	Koc = 1887; logKoc = 3,276

PNEC calculation Assessment factors

Data availability	Assessment factor
At least one short-term L(E)C₅₀ from each of three trophic levels of the base-set (fish, Daphnia and	1000
One long-term NOEC (either fish or Daphnia)	100
Two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae)	50
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10
Field data or model ecosystems	Reviewed on a case by case basis

calculations PNECaquatic

RBT = Ready biodegradability test

NT = No toxic

- = No test data

mg/l	Chemical 1	Chemical 2	Chemical 3	Chemical 4	Chemical 5
Water solubility	1000	10000	10	1000	0.5
EC ₅₀ Daphnia	100	500	3	200	10
EC ₅₀ Algae	50	1000	0.1	500	20
EC ₅₀ Fish	90	NT	0.16	-	50
NOEC Daphnia	-	100	0.1		5
NOEC Fish	-	-	-	-	3
NOEC Algae	-	-	0.01	-	2
Log Kow	1	-	6	-	-
BCF	-	50	-	110	5
RBT	Yes	Yes	No	Yes	Yes
Classification					
PNECaquatic					
Further testing					