Summary of Initial Risk Assessment Report

Ethylbenzene CAS No : 100-41-4

PRTR No of Japan: 40

This substance is assessed based on Guideline for Initial Risk Assessment Version 2.0

1. General Information

1.1 Physico-chemical properties

Appearance	Colorless liquid
Melting point	-95.01 degC
Boiling point	136.25 degC
Water solubility	152 mg/L (20 degC)
Henry's constant	798 Pa*m^3/mol ($7.88*10^{-3}$ atm*m^3/mol) (25degC, measured)
Octanol/water partition coefficient (log Kow)	3.15 (measured), 3.03 (estimated)
Soil adsorption coefficient	Koc = 164 (measured)

1.2 Environmental fate

Bioaccumulation	Low bioaccumulative Bioconcentration factor (BCF): log BCF 1.9 (goldfish), 0.67 (Clam) , measured
Biodegradation	Readily biodegradable Considered to be biodegraded also under anaerobic conditions after a long lag phase.
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is $7.1*10^{-12}$$cm^3$/molecule-sec. (25 degC, measured) The half-life is 1-2 days, given OH radical concentration of $5*10^5$ – $1*10^6$ molecule/cm^3. Reaction with ozone: No data Reaction with nitrate radical: Reaction rate constant is $5.7*10^{-16}$$cm^3$/molecule-sec. (25 degC, measured) The half life is 0.2-2 months, given nitrate radical concentration of $2.4*10^8$ - $2.4*10^9$ molecule/cm^3 (10 - 100ppt). (In water) Not expected to hydrolyze in water.
Environmental fate	If released into water, ethylbenzene is expected to be removed by biodegradation easily under aerobic conditions and is also expected to be removed by biodegradation after a long lag period under anaerobic conditions . It is also expected to be removed by volatilization

2. Sources of release to the environment

2.1 Annual production, import, export and domestic supply in 2003 (ton/year)

Production	Import	Export	Domestic supply	Remarks
3,490,218	< 0.5	218	3,490,000	--

2.2 Uses

The main use is raw material of the styrene monomers.

2.3 Release from the industries within the scope of PRTR system (in 2003)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	12,674	3	< 0.5	Release to rivers: 19 tons
	Release outside notification	4,470	< 0.5	0	
Release outside notification from non listed industry		6,295	18	55	
Households		558	0	< 0.5	
Mobile sources		6,573	0	0	
Total		30,570	21	55	

2.4 Releases from other sources

No information is available.

2.5 Main release route

According to 2003 PRTR data and other information about the use of ethylbenzene in solvents, ethylbenzene is expected to be released to air mainly during use of solvents for paints and through vehicle engine emissions.

3. Exposure Assessment

3.1 Measured environmental concentration

Media	No. of points detected / No. of points measured	No. of samples detected / No. of samples measured	Detection range	95th percentile	Detection limit	Year of investigation, Institution
Air (microg/m^3)	--	--/201	0.100 - 501.9	70	--	1998 Ministry of Health and Welfare
River water (microg/L)	12/124	12/124	nd-0.47	0.020	0.01	1999 Ministry of the Environment
Sea water (microg/L)	1/20	1/20	nd-0.01	0.0053	0.01	1999 Ministry of the Environment
Drinking water (microg/L)(as ground water)	2/23	2/23	nd-0.15	0.028	0.01	1999 Ministry of the Environment
Food (microg/g) (fish)	16/42	43/138	nd-0.0098	0.0050	0.001	1986 Ministry of the Environment

nd: Not detected

For calculation of the 95th percentile, data less than the detection limit are replaced with a value equal to 1/2 of the detection limit.

3.2 Estimated environmental concentration

Media	Estimated concentration	Description
Air (microg/m^3)	9.3	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) Ver.1.5
River water (microg/L)	0.75	Calculated by mathematical model / Integrated River Model to predict the distribution of chemical concentration (IRM1)

3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	0.75
	Estimated concentration by model (0.75 microg/L) was used for the risk assessment, since the value is higher than measured concentration. [1)].

3.4 Estimated human intake

Intake route		Concentration used for estimation of intake	Estimated intake (microg/ person/day)	Estimated intake (microg/ kg-Bodyweight (BW)/day)
Inhalation	Air	70 (microg/m^3)	690	14
		Concentrations of ethylbenzene in indoor air were higher than those in outdoor air. The 95 percentile of measured concentrations in indoor air was used for the risk assessment, since the value was higher than estimated concentration in air by model. [1)] An absorption rate of ethyl benzene through human breathing was reported to be 49%. Based on this ratio, intakes from inhalation route were estimated to be 690 microg/ person/day and 14 microg/ kgBW/day.		
Oral	Drinking water	0.028 (microg/L)	0.056	0.0011
		Concentration in ground water was used as a substitute, since no measured concentration in tap water was available. The 95th percentile of concentrations in ground water was used.		
	Food	0.00042 (microg/g)	0.050	0.001
		-Data of intake via food were not available. -Concentration in fish body was estimated as a product of a concentration in sea water and a BCF. -The 95th percentile value (0.0053 microg/L) of measured concentrations in the survey by the Ministry of the Environment in 1999 was used for concentration in sea water.		
	Subtotal	--	0.11	0.0021
Total route		--	690	14

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version2.0. Under Version 2.0, a measured concentration and an estimated concentration (calculated by mathematical model) are compared and the larger of two concentrations is used for risk assessment.

4. Hazard assessment

4.1 Effects on organisms in the environment

	Acute or Chronic	Species	Endpoint	Concentration
Algae	Acute	*Selenastrum capricornutum*	96 hours EC_{50} Growth inhibition	3.6 (mg/L)
Crustacea	Chronic	*Ceriodaphnia dubia*	7 days NOEC Reproduction	1.0 (mg/L)
Fish	Acute	*Oncorhynchus mykiss*	96 hours LC_{50}	4.2 (mg/L)
Key study		Data of crustacea (a kind of *Ceriodaphnia dubia*) was chosen for the key study because effects were observed at the lowest concentration in the hazard assessment.		

4.2 Human health toxicity

Toxicity	Exposure route	Species	Duration / Dose method	Toxic effects (Key study is underlined)	NOAEL or LOAEL (converted)
Repeated dose toxicity	Inhalation	Rat	2 years	Nephropathy in females, prostate gland inflammation in males, renal tubule hyperplasia, mineralization of blood vessel walls and stomach in males, and bone marrow hyperplasia in males	LOAEL: 75 ppm (330 mg/m^3) (equivalent to 19 mg/kg/day)
	Oral	Rat	6 months Gavage	Increased absolute weight of liver and kidneys, cloudy swelling of hepatocytes and renal tubular epithelium cells	NOAEL: 136 mg/kg/day (equivalent to 97 mg/kg/day)
	Dermal	--	--	--	--
Reproductive and developmental toxicity	--	The reproductive effect and fetal toxicant cannot be evaluated			
Carcinogenicity	Inhalation	Rat	2 years Inhalation	Tumour of kidney in female/male	NOAEL: 250 ppm (equivalent to 64 mg/kg/day)
	Evaluation by IARC: Group 2B (possibly carcinogenic to humans)				
Genotoxicity	Not considered genotoxic				

5. Risk Assessment

5.1 Environmental organisms

	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
Risk characterization	0.75	NOEC:1.0	1,300	100	No immediate concern
	Product of uncertainty factors (UF): Extrapolation from laboratory test (10) *Extrapolation from chronic toxicity data on one trophic level (10) = 100				
Recommendation : --					

NOEC* means NOEC, LOEC, EC_{50}, etc.

5.2 Human health

5.2.1 Repeated dose toxicity

Exposure route	Intake (microg/kgBW/day)	NOAEL (mg/kgBW/day)	Risk characterization		
			MOE	Product of uncertainty factors	Conclusion
Inhalation	14	LOAEL: 19	1,400	1,000	No immediate concern
Oral	0.0021	97	46,000,000	200	No immediate concern
Total	--	--	--	--	--
Product of uncertainty factors (UF): Inhalation: Interspecies (10) * Intraspecies (10) * Using LOAEL (10) = 1,000 Oral: Interspecies (10) * Intraspecies (10) * Duration of test (2) = 200					

5.2.2 Reproductive and developmental toxicity

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5.2.3 Carcinogenicity

Exposure route	Intake (microg/kgBW/day)	NOAEL (mg/kgBW/day)	Risk characterization		
			MOE	Product of uncertainty factors	Conclusion
Inhalation	14	64	4,600	1,000	No immediate concern
Product of uncertainty factors (UF): Interspecies (10) * Intraspecies (10) * Carcinogenicity(10) = 1,000					

5.2.4. Recommendation for Human Health

The substance is considered to be of no immediate concern for the moment, and low priority for further work.

6. Supplement

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