Summary of Initial Risk Assessment Report

Isoprene CAS No : 78-79-5

PRTR No of Japan: 28

This substance is assessed based on Guideline for Initial Risk Assessment Version 1.0

1. General Information

1.1 Physico-chemical properties

Appearance	Colorless liquid
Melting point	-145.95 (degC)
Boiling point	34.067 (degC)
Water solubility	300 mg/L (20 degC)
Henry's constant	7.77 Pa*m^3/mol ($7.67*10^{-2}$ atm*m^3/mol) (25degC, measured)
Octanol/water partition coefficient (log Kow)	l2.42 (measured), 2.58 (estimated)
Soil adsorption coefficient	Koc = 68 (estimated)

1.2 Environmental fate

Bioaccumulation	Exhibits little to no bioaccumulation. Bioconcentration factor (BCF) : 5.0 - 14 (50 microg/L)/<5.6-20 (5 microg/L) (Carp) measured
Biodegradation	Non-biodegradable
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is $1.0*10^{-10}$ cm^3/molecule/sec. (25 degC, measured) The half-life is 2 - 4 hours, given OH radical concentration of $5*10^5$ – $1*10^6$ molecule/cm^3. Reaction with ozone: Reaction rate constant is $1.4 * 10^{-17}$ cm^3/molecule-sec. (25 degC, measured) The half - life is 20 hours, given ozone concentration of $7 * 10^{11}$ molecule/cm^3. Reaction with nitrate radical: Reaction rate constant is $6.8 * 10^{-13}$ cm^3/molecule-sec. (25 degC, measured) The half - life is 7 - 70 minutes, given nitrate radical concentration of $2.4 * 10^8$ - $2.4 * 10^9$ molecule/cm^3 (10 - 100 ppt). (In water) Not expected to hydrolyze in water
Environmental fate	If released into water, isoprene is expected to be removed mainly by volatilization.

2. Sources of release to the environment

2.1 Annual production, import, export and domestic supply in 2001 (ton/year)

Production	Import	Remarks
62,000		If the percentages of isoprene in polyisoprene rubber and butyl rubber are 100% and 5% respectively, the sum of the production and import of isoprene is estimated to be 62,000 tons in 2001.

2.2 Uses

Raw material for polyisoprene rubber (93%), raw material for butyl rubber (7%)

2.3 Release from the industries within the scope of PRTR system (in 2001)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	122	0	0	
	Release outside notification	0.001	0	0	
Release outside notification from non listed industry		--	--	--	Release to river: 0
Households		--	--	--	
Mobile sources		--	--	--	
Total		122	0	0	

2.4 Releases from other sources

It has been reported that possible sources of isoprene are plants, tobacco smoke, and worn rubber. The releases from plants and worn tires were not included in 2001 PRTR data.

2.5 Main release route

Isoprene is expected to be released mainly through the manufacture of synthetic rubber. The releases from plants, tobacco smoke, and worn rubber were not considered in this assessment because they could not be estimated.

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)	2/3	--	nd-0.23	--	0.17	1995 Ministry of the Environment
River water (microg/L)	1/44	--	nd-0.02	0.005	0.01	2000 Ministry of the Environment
Sea water (microg/L)		0/11	nd	-	0.01	2000 Ministry of the Environment
Drinking water (microg/L)(as ground water)	2/15	--	nd-0.03	0.016	0.01	2000 Ministry of the Environment
Food (microg/g)	--	0/45	--	--	0.005	1999 Japan Food Research Laboratories

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)	0.62	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) ver.1.0
River water (microg/L)	0	Concentration in river water is estimated to be 0 microg/L, since no release to river due to 2001 PRTR data.

3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	0.005
	The 95th percentile (0.005 microg/L) of measured concentrations in the survey by the Ministry of the Environment was used for the risk assessment[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	0.62 (microg/m^3)	12.4	0.25
		Estimated concentration was used because the number of the samples in the survey by the Ministry of the Environment was not enough.		
Oral	Drinking water	0.0160 (microg/L)	0.032	0.00064
		The ninety-fifth percentile of measured concentrations in ground water were used, since measured concentrations in drinking water were not available.		
	Food	0.0001 (microg/g)	0.012	0.00024
		-Isoprene was not detected in any samples in the survey by the Ministry of the Environment in 2000 (detection limit: 0.01 microg/L). - Therefore the concentration in foods was estimated as concentration in fish. -The concentration in fish was estimated as a product of the concentration in seawater and a BCF.		
	Subtotal	--	0.044	0.00088
Total route		--	12.4	0.25

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version1.0. If adequate measured concentrations are available, they are given priority and used as values for risk assessment. If they are not available, an estimated value calculated using a mathematical model is used.

4. Hazard assessment

4.1 Effects on organisms in the environment

Species	Acute or Chronic	Species	Endpoint	Concentration
Algae	Chronic	*Selenastrum capricornutum*	72 hours NOEC Growth inhibition, Biomass	82.7 (mg/L)
Crustacea	Chronic	*Daphnia magna*	21 days NOEC Reproduction	0.402 (mg/L)
Fish	Acute	*Oryzias latipes*	96 hours LC_{50}	14.8 (mg/L)
Key study		Data of crustacea (*Daphnia magna*) 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
Repeated dose toxicity	Inhalation	Mouse	26 weeks	abnormal posture and hindlimb dysfunction, <u>spinal cord degeneration</u>, testicular atrophy, degeneration of olfactory epithelium and hyperplasia of squamous epithelium in forestomach	LOAEL 70 ppm (equivalent to 59 mg/kg/day)
	Oral	--	--	--	--
	Dermal	--	--	--	--
Reproductive and developmental toxicity	Inhalation	Reduced maternal body weight gain, decreased fetal body weight and fetal skeletal alterations (extra ribs) in mice, and delayed ossification of centrum in rat fetuses NOAEL for dam: 1,400 ppm, LOAEL for developmental toxicity: 280 ppm			
Carcinogenicity	Evaluation by IARC: Group 2B (possibly carcinogenic to humans)				
Genotoxicity	Considered to be genotoxic				

5. Risk Assessment

5.1 Environmental organisms

Risk characterization	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
	0.005	NOEC: 0.402	80,000	500	No immediate concern
	Product of uncertainty factors (UF): Extrapolation from laboratory test (10) * Toxicity data on two nutritional stages (5) = 500				
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	0.25	LOAEL: 59.0	240,000	2,000	No immediate concern
Oral	0.00088	No adequate data	Not calculated	Not calculated	Could not be assessed
Total	--	--	--	--	--
Product of uncertainty factors (UF): Inhalation: Interspecies (10) * Intraspecies (10) * Using LOAEL(10) * Duration of test (2) = 2,000					

5.2.2 Reproductive and developmental toxicity

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5.2.3 Carcinogenicity

Risk characterization of carcinogenicity of the substance was not carried out in this assessment.

5.2.4. Recommendation for Human Health

Though the substance is considered to be of no immediate concern for the moment and a low priority for further work, it should be noted that a carcinogenic risk characterization was not conducted. The possibility remains that this substance may be carcinogenic to humans. As for oral exposure, a risk assessment was not conducted due to a lack of toxicity data.

6. Supplement

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