Summary of Initial Risk Assessment Report

Allyl alcohol CAS No : 107-18-6

PRTR No of Japan: 22

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	-50 degC
Boiling point	96 - 97 degC
Water solubility	Miscible
Henry's constant	0.505 Pa*m^3/mol (4.99*10^{-6} atm*m^3/mol) (25degC, estimated)
Octanol/water partition coefficient (log Kow)	0.17 (measured), 0.21 (estimated)
Soil adsorption coefficient	Koc = 1 (estimated)

1.2 Environmental fate

Bioaccumulation	Low bioaccumulative Bioconcentration factor (BCF): 3.16 (calculated using logKow of 0.17)
Biodegradation	Readily biodegradable Considered to be biodegradable substance under aerobic and anaerobic conditions.
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is 4.3*$10^{-11}$$cm^3$/molecule-sec. (25 degC, measured). The half-life is 4 - 9 hours, given OH radical concentration of 5*10^5 – 1*10^6 molecule/cm^3. Reaction with ozone: Reaction rate constant is 1.44*$10^{-17}$$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 1.30*$10^{-14}$$cm^3$/molecule-sec. (25 degC, measured) The half life is 0.3 - 3 days, 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 Allyl alcohol has been reported that 13.9% of the solution at 50 degC is photodegraded to carbon dioxide by the exposure to ultraviolet radiation for 24 hours.
Environmental fate	If released into water, volatilization from water surfaces is expected to be low.

2. Sources of release to the environment

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

Production	Import	Export	Domestic supply	Remarks
45,000	--	--	--	--

2.2 Uses

Raw material for allyl-glycidyl ether and epichlorohydrin, raw material for synthetic resins such as diallyl phthalate resins, raw material for medicine, perfume and flame retardant.

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

Release sources		Air (ton)	Water (ton)	Soil (ton)	Remarks
Listed industries	Reported release	49	8	0	Release to rivers: 1.32 tons
	Release outside notification	--	--	--	
Release outside notification from non listed industry		--	--	--	
Households		--	--	--	
Mobile sources		--	--	--	
Total		49	8	0	

2.4 Releases from other sources

No information about the substance is available

2.5 Main release route

Allyl alcohol is expected to be released into the environment mainly during use of the substance or products containing it.

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)	1/5	3/15	nd - 0.06	0.053	0.01 - 0.03	1995 Ministry of the Environment
River water (microg/L)	0/44	--	nd	--	0.3	2000 Ministry of the Environment
Sea water (microg/L)	0/11	--	nd	--	0.3	2000 Ministry of the Environment
Drinking water (microg/L) (as groundwater)	0/15	--	nd	--	0.3	2000 Ministry of the Environment
Food	--	--	--	--	--	--

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)	0.802	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) ver.1.0
River water (microg/L)	0.304	Calculated by mathematical model / Initial Assessment System for the PRTR chemicals (IAS)

3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	0.15
	The value (0.15 microg/L) equal to 1/2 of detection limit was used for the risk assessment, since allyl alcohol was not detected in the survey by the Ministry of the Environment[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	0.053 (microg/m^3)	1.1	0.021
		The 95th percentile of measured concentrations (0.053 microg/m^3) was used for the risk assessment.		
Oral	Drinking water	0.15 (microg/L)	0.30	0.006
		-Since data of tap water were not available, measured concentrations in ground water were used. -The value (0.15 microg/L) equal to 1/2 of detection limit (0.3 microg/L) was used for the risk assessment, since allyl alcohol was not detected in any samples.		
	Food	0.00047 (microg/g)	0.057	0.0011
		-Data of intake via food were not available. -Concentration in fish body is estimated as a product of an estimated concentration in seawater and a BCF. -The value equal to 1/2 of detection limit is used for seawater concentration, since allyl alcohol was not detected in any samples.		
	Subtotal	--	0.36	0.0071
Total route		--	1.4	0.028

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 the 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

	Acute or Chronic	Species	Endpoint	Concentration
Algae	Chronic	*Selenastrum capricornutum*	72 hours NOEC Growth inhibition (Growth rate)	9.69 (mg/L)
Crustacea	Chronic	*Daphnia magna*	21 days Reproduction	0.919 (mg/L)
Fish	Acute	*Pimephales promelas*	96 hours LC_{50}	0.32 (mg/L)
Key study		Data of fish (*Pimephamelas promelas*) is 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	Rat	12 weeks	Reduced body weight gains, increased relative weight of lung and kidneys	NOAEL: 5 ppm (12.1 mg/m^3) (equivalent to 1.87 mg/kg/day)
	Oral	Rat	15 weeks Drinking water	Increased absolute and relative weight of kidneys, Increased relative weight of liver and spleen, reduced body weight gains	NOAEL50 ppm (6.2 mg/kg/day)
	Dermal	--	--	--	--
Reproductive and developmental toxicity	On the test in mating between the male rat with oral administration and the female rat with non-treated, considered not to be influence in the reproductive function.				
Carcinogenicity	Evaluation by IARC : This substance has not been evaluated by IARC.				
Genotoxicity	Unable to determine genotoxicity				

5. Risk Assessment

5.1 Environmental organisms

	EEC (microg/L)	NOEC* (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
Risk character -ization	0.15	LC_{50}: 0.32	2,100	1,000	No immediate concern
	Product of uncertainty factors (UF): Extrapolation from laboratory test (10) * Acute toxicity test (100) = 1,000				
Recommendation : The substance is considered to be of no immediate concern for the moment, and low priority of further work.					

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 (NOAEL / intake)	Product of uncertainty factors	Conclusion
Inhalation	0.021	1.87	89,000	500	No immediate concern
Oral	0.0071	6.2	870,000	500	No immediate concern
Total	0.028	1.87 (Inhalation)	67,000	500	No immediate concern
Product of uncertainty factors (UF): Inhalation/Oral/Total: Interspecies (10) * Intraspecies (10) * Duration of test (5) = 500					

5.2.2 Reproductive and developmental toxicity

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5.2.3 Carcinogenicity

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5.2.4. Recommendation for Human Health

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

6. Supplement

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