

Summary of Initial Risk Assessment Report

1-Octanol CAS No : 111-87-5

PRTR No of Japan: 58

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	- 16 degC
Boiling point	194 to 195 degC
Water solubility	300 mg/L (20 degC), 540 mg/L (25degC)
Henry's constant	2.48 Pa*m ³ /mol (2.45*10 ⁻⁵ atm*m ³ /mol) (25degC, measured)
Octanol/water partition coefficient (log Kow)	3.00 (measured), 2.81 (estimated)
Soil adsorption coefficient	Koc = 28 (estimated)

1.2 Environmental fate

Bioaccumulation	Low bioaccumulative Bioconcentration factor (BCF): 41 (calculated using logKow of 3.00)
Biodegradation	Readily biodegradable Considered to be biodegradable under anaerobic conditions although the process is slow.
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is 1.30*10 ⁻¹¹ cm ³ /molecule-sec (25degC, estimated). The half - life is 0.6 - 1 day, given OH radical concentration of 5*10 ⁵ – 1*10 ⁶ molecule/cm ³ . Reaction with ozone: No data Reaction with nitrate radical: No data The substance is not expected to photodegrade directly. (In water) Hydrolysis is not expected to occur in the aquatic environment, since this substance lacks functional groups that hydrolyze under environmental conditions.
Environmental fate	If released into water, 1-Octanol is expected to be removed mainly by biodegradation and partially by volatilization.

2. Sources of release to the environment

2.1 Annual production, import, export and domestic supply in 2002 (ton/year)

Production	Import	Export	Domestic supply	Remarks
500	2,500	0	3,000	--

2.2 Uses

Raw materials: stabilizer (organotin reagent) (50%), plasticizer (di-*n*-octylphthalate) (35%), and rose jasmine perfume(15%).

2.3 Release from the industries within the scope of PRTR system (in 2004)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	2.4	0.037	0	Released into river: 0.038 ton
	Release outside notification	0.069	0.001	0	
Release outside notification from non listed industry		--	--	--	
Households		--	--	--	
Mobile sources		--	--	--	
Total		2.5	0.038	0	

2.4 Releases from other sources

No information is available.

2.5 Main release route

Based on 2004 PRTR data and known uses of the substance, 1-octanol is expected to be released into air mainly during its use in electrical machinery and equipment manufacturing industries and chemical industries.

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	--	--	--	--	--	--
River water (microg/L)	44/44	44/44	0.004-0.54	0.17	0.002	2001 Ministry of the Environment
Sea water (microg/L)	8/14	24/42	nd-0.046	0.018	0.0007- 0.002	2002 Ministry of the Environment
Drinking water	--	--	--	--	--	--
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)	0.019	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) Ver.1.5
River water (microg/L)	0.0052	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)	0.17
	The measured concentration in river water was used for the risk assessment, since the value is higher than the value estimated by model 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	0.019 (microg/m ³)	0.38	0.0076
	The estimated concentration of 0.019 microg/ m ³ was used for the risk assessment, since no measured concentration was available			
Oral	Drinking water	0.17 (microg/L)	0.34	0.0068
	Concentration in river water was used, since neither measured concentrations in tap water nor in ground water were available. The 95th percentile of measured concentrations was used for the risk assessment.			
	Food	0.00074 (microg/g)	0.089	0.00178
	Data of intake via food were not available. Concentration in fish was estimated as a product of the 95th percentile of concentrations in seawater and a BCF.			
	Subtotal	--	0.429	0.0086
Total route		--	0.429	0.016

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version 2.0. 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	<i>Scenedesmus subspicatus</i>	48 hours EC ₅₀ Growth inhibition, Growth rate	4.2 (mg/L)
Crustacea	Chronic	<i>Daphnia magna</i>	21 days NOEC Reproduction	1.0 (mg/L)
Fish	Acute	<i>Pimephales promelas</i>	7 days NOEC Growth	0.75 (mg/L)
Key study		Fish (<i>Pimephales promelas</i>) 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	--	--	--	No data
	Oral	--	--	--	No data
	Dermal	--	--	--	No data
Reproductive and developmental toxicity	Oral	Rat	GD 6-15 Oral	No teratogenic and Reproductive/developmental effects at dose at dose level of dam toxicity observed	--
Carcinogenicity	Evaluation by IARC : This substance has not been evaluated by IARC.				
Genotoxicity	Unable to determine genotoxicity				

5. Risk Assessment

5.1 Environmental organisms

Risk characterization	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
	0.17	NOEC:0.75	4,400	1,000	No immediate concern
Product of uncertainty factors (UF): Extrapolation from laboratory test (10) * Extrapolation from acute toxicity test (100) = 1,000					
Recommendation : --					

NOEC* means NOEC, LOEC, EC₅₀, 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	0.0076	No data	--	--	--
Oral	0.0086	No data	--	--	--
Total	0.016	--	--	--	--
Product of uncertainty factors (UF): --					

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 risk assessment could not be conducted because adequate toxicity data was not available. A risk assessment should be conducted when toxicity data becomes available.

6. Supplement

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