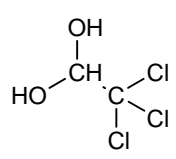| 4	CAS No.: 302-17-0	Substance: 2,2,2-Trichloroethane-1,1-diol

Chemical Substances Control Law Reference No.:

PRTR Law Cabinet Order No.:

Molecular Formula: $C_2H_3Cl_3O_2$ Structural Formula:

Molecular Weight: 165.40

1. General information

The aqueous solubility of this substance is 9.31×10^6 mg/L (38°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 0.99, and the vapor pressure is 15.0 mmHg (=2.0×10^3 Pa) (25°C). Data could not be obtained for biodegradability (aerobic degradation). This substance hydrolyzes at high pH levels to form chloroform.

The main use of this substance is as a raw material for pharmaceutical ingredients. The production quantity in fiscal 2009 was approximately 5 t.

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2. Exposure assessment

This substance is formed by the hydration of trichloroacetaldehyde. Total release of trichloroacetaldehyde to the environment in fiscal 2010 under the PRTR Law was 1.5 t, and all releases were reported. All releases were to public seawater bodies. The only source of reported releases was the chemical industry. Predictions of proportions distributed to individual media by using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the predicted proportions distributed to water bodies and soil were greater.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained. However, the PEC was 3 µg/L at maximum in freshwater bodies on the basis of measurements of raw water from the surface of lakes, including dam lakes.

3.Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC_{50} in excess of 95,400 µg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*, a 48-h EC_{50} in excess of 97,700 µg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} in excess of 95,900 µg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) in excess of 950 µg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 14,700 µg/L for growth inhibition in the green alga *P. subcapitata*, and a 21-d NOEC of 11,500 µg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 120 µg/L was obtained.

The value of 120 µg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The risk of this substance could not be judged because data for setting the predicted environmental concentration (PEC) could not be obtained. Assuming that the PEC for this substance is set at 3 µg/L for

freshwater bodies on the basis of the measurements of raw water from the surfaces of lakes, including dam lakes, its ratio to PNEC is less than 0.1. Accordingly, further work is considered unnecessary at this time.

Hazard assessment (basis for PNEC)			Assessment factor	Predicted no effect concentration PNEC (µg/L)	Exposure assessment		PEC/PNEC ratio	Judgment based on PEC/PNEC ratio	Assessment result
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (µg/L)			
Crustacean *Daphnia magna*	Chronic	NOEC Reproductive inhibition	100	120	Freshwater			×	
					Seawater				

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4. Conclusions

	Conclusions	Judgment
Ecological risk	No need of further work at present.	

Risk judgments   : No need for further work   ▲: Requiring information collection

   ■: Candidates for further work   ×: Impossibility of risk characterization

   : Though a risk characterization cannot be determined, there would be little necessity of collecting information.

   : Further information collection would be required for risk characterization.