4	CAS No. 96-23-1	Substance: 1,3-Dichloro-2-propanol

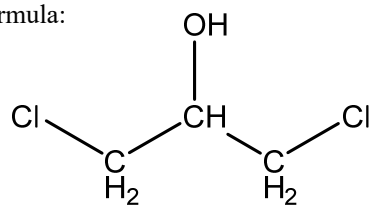
Chemical Substances Control Law Reference No.: 2-2002 (Mono (or di, or tri) bromo (or chloro) alkanol (C = 2–5)

PRTR Law Cabinet Order No.: 2-36

Molecular Formula: $C_3H_6Cl_2O$

Molecular Weight: 128.99

Structural Formula:



1. General information

The aqueous solubility of this substance is 9.9×10^4 mg/L (19°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 0.2, and the vapor pressure is 0.750 mmHg (=100Pa) (21.8°C). Biodegradability (aerobic degradation) is judged to be good. The half-life for hydrolysis is 9.1 d (pH = 7, 25°C).

This substance is classified as a Class 2 Designated Chemical Substance under the PRTR Law. The main uses of this substances are as a cellulose-based material cross-linking agent, synthetic resin solvent, raw material for epichlorohydrin etc., dyestuff auxiliary, and as a wet strength agent for paper. The production and import quantity in fiscal 2017 was less than 1000 t. The production and import category under the PRTR Law is more than 1 t and less than 100 t.

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2. Exposure assessment

This substance was classified as a Class 1 Designated Chemical Substance prior to revision of substances regulated by the PRTR Law. Total release to the environment in fiscal 2009 under the PRTR Law was approximately 200 t, of which approximately 21 t or 10% of overall releases were reported. The major destination of reported releases was public water bodies. In addition, approximately 6.2 t was transferred to waste materials and approximately 10 t was transferred to sewage. Industries with large reported releases were the pulp & paper and paper products manufacturing industries and the textile industry. The largest releases to the environment including unreported releases were to water bodies. A multimedia model used to predict the proportions distributed to individual media in the environment indicated that in regions where the largest quantities were estimated to have been released to the environment overall or the atmosphere and public water bodies in particular in fiscal 2009, the predicted proportion distributed to public water bodies would be 99.0%.

The maximum expected concentration of exposure to humans via inhalation, based on ambient atmospheric data, was around 0.0037 μg/m^3. However, because this substance was removed from the Class 1 Designated Chemical Substance list as a result of the revision of substances regulated by the PRTR Law, the mean annual value for the atmospheric concentration was calculated by using a plume-puff model based on releases to the atmosphere using the most recent available data from fiscal 2009: this model predicted a maximum level of 0.74 μg/m^3.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. In lieu of such data, the maximum expected exposure was calculated to be around 0.021 μg/kg/day assuming intake solely from public freshwater bodies. Further, a maximum expected concentration of exposure of around 1.2 μg/kg/day was calculated from past data for public freshwater bodies. In addition, albeit based on past data, when releases reported under the PRTR Law in fiscal 2009 to public freshwater bodies estimated from the reported transfer to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 86 μg/L. Calculating oral exposure based on this gives 3.4 μg/kg/day.

The risk of exposure to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on the basis of its physicochemical properties. Further, this substance (1,3-DCP), 3-chloropropane-1,2-diol (3-MCPD), and other chloropropanols are known to be used in processes to manufacture acid-hydrolyzed plant proteins via hydrolysis of plant proteins using hydrochloric acid.

In terms of chloropropanol concentration in soy sauce made using the mixed brewing method or mixed method, the

lower the concentration of 3-MCPD, the lower the concentration of 1,3-DCP becomes, and because 3-MCPD concentration has been confirmed to be low, the 1,3-DCP concentration is also thought to be low.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was reported to be around 0.53 μg/L for public freshwater bodies and around 0.07 μg/L for seawater. Further, past data for public freshwater bodies and seawater indicated values of around 29 μg/L and around 0.13 μg/L, respectively. When releases reported under the PRTR Law in fiscal 2009 to public freshwater bodies estimated from the reported transfer to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 86 μg/L.

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3. Initial assessment of health risk

This substance causes toxic symptoms similar to carbon tetrachloride poisoning, but its irritation effects (for example, hemorrhagic gastritis, pharyngitis, etc.) may be more severe.

As sufficient information on the carcinogenicity of the substance was not available, the initial assessment was conducted on the basis of information on its non-carcinogenic effects.

The NOAEL of 1 mg/kg/day for oral exposure (based on increase in liver weight), determined from toxicity tests in rats, was adjusted according to exposure conditions to obtain 0.7 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.07 mg/kg/day was deemed to be the lowest reliable dose and was identified as the 'non-toxic level' of the substance for oral exposure. The 'non-toxic level' for inhalation exposure could not be identified.

With regard to oral exposure, assuming the substance is absorbed via public freshwater bodies, the predicted maximum exposure level would be 0.021 μg/kg/day, approximately. The MOE (Margin of Exposure) would be 67, when calculated from the predicted maximum exposure level and the 'non-toxic level' of 0.07 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans and by another factor of 5 to take into consideration the carcinogenicity in animals. This would lead to the health risk judgment that collection of information would be required. In addition, the MOE for reference would be 0.4, when calculated from the estimated maximum exposure level of 3.4 μg/kg/day. This maximum exposure level was estimated according to old data reported in FY 2009 under the PRTR Law on the concentration in effluents from the high discharging plants. Since exposure to the substance in environmental media via food is presumed to be limited in spite of data unavailability, including it in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, collection of information would be required to assess the health risk of this substance via oral exposure, starting from data on water quality near the high discharging plants.

With regard to inhalation exposure, owing to the lack of identified 'non-toxic level, the health risk could not be assessed. However, the MOE would be 1,200, when calculated from the tentative 'non-toxic level' for inhalation exposure of 0.23 mg/m^3 and the predicted maximum exposure concentration in ambient air of 0.0037 $\mu g/m^3$ approximately, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans and by another factor of 5 to take into consideration the carcinogenicity in animals. The tentative 'non-toxic level' for inhalation exposure above was derived from the conversion of the 'non-toxic level' for oral exposure, assuming that 100% of the inhaled substance is absorbed. On the other hand, the MOE for reference would be 6, when calculated from the concentration of 0.74 $\mu g/m^3$. This concentration was estimated as the maximum concentration (annual mean) in ambient air near the operators releasing large amount of this substance based on old data on the releases to air reported in FY 2009 under the PRTR Law. Therefore, as a comprehensive judgment, collection of information would be required to assess the health risk of this substance via inhalation in ambient air, starting from data on concentrations in ambient air near the operators releasing large amount of this substance.

Toxicity				Exposure assessment		MOE		Comprehensive judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure dose and concentration			
Oral	'Non-toxic level' 0.07 mg/kg/day	Rats	Increase in liver weight, etc.	Drinking water	- μg/kg/day	MOE	-	▲
				Public Freshwater bodies	0.021 μg/kg/day	MOE	67	
Inhalation	'Non-toxic level' - mg/m^3	-	-	Ambient air	0.0037 $\mu g/m^3$	MOE	-	▲
				Indoor air	- $\mu g/m^3$	MOE	-	×

Non-toxic level *

- When a LOAEL is available, it is divided by 10 to obtain a NOAEL-equivalent level.
- When an adverse effect level for the short-term exposure is available, it is divided by 10 to obtain a level equivalent to an adverse effect level for the long-term exposure.

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4. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC_{50} exceeding 100,000 μg/L for growth inhibition in the green alga *Raphidocelis subcapitata*, a 48-h LC_{50} of 725,000 μg/L for swimming inhibition in the crustacean *Daphnia magna*, a 96-h LC_{50} exceeding 100,000 μg/L for the fish species *Oryzias latipes* (medaka), and a 96-h LC_{50} exceeding 100,000 μg/L for the fish species *Cyprinus carpio* (carp). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 7250 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-d NOEC of 34,800 μg/L for growth inhibition in the green alga *R. subcapitata* and a 21-d NOEC of 6250 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 62 μg/L was obtained.

The value of 62 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio is 0.009 for freshwater bodies and 0.001 for seawater; accordingly, further work to determine the ecological risk is considered unnecessary at this time.

However, past data, albeit obtained from a survey of a limited area, indicate maximum values of around 29 μg/L for public freshwater bodies and around 0.13 μg/L for seawater. The ratios to the PNEC are 0.5 for freshwater and 0.002 for seawater. In addition, when releases reported under the PRTR Law in fiscal 2009 to public freshwater bodies estimated from the reported transfer to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 86 μg/L. The ratio of this value to the PNEC is 1.4; accordingly, based on a comprehensive review of the above findings, efforts to collect data are needed, and environmental concentration data needs to be augmented taking into consideration major emission sources based on the production and import quantity and trends in emissions to the environment.

Hazard assessment (basis for PNEC)			Assessment coefficient	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Comprehensive judgment
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacean *Daphnia magna*	Chronic	NOEC Reproductive inhibition	100	62	Freshwater	0.53	0.009	▲
					Seawater	0.07	0.001	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Requiring information collection.	▲
	Inhalation exposure	Requiring information collection.	▲
Ecological risk	Requiring information collection.		▲

［Risk judgments］○: No need for further work ▲: Requiring information collection
■: Candidates for further work ×: Impossibility of risk characterization