2	CAS No. 79-11-8	Substance: Chloroacetic acid

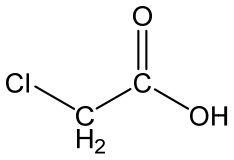
Chemical Substances Control Law Reference No.: 2-1145

PRTR Law Cabinet Order No.: 98

Molecular Formula: $C_2H_3ClO_2$

Molecular Weight: 94.50

Structural formula:



1.General information

The aqueous solubility of this substance is 6.14×10^6 mg/1000 g (25°C), the partition coefficient (1-octanol/water) (log Kow) is 0.22 (pH unknown), and the vapor pressure is 8.67 Pa (25°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 65%, and biodegradability is judged to be good. In addition, the half-life for hydrolysis is 960 days.

From the perspectives of human health and ecological effects, this substance is designated as a Priority Assessment Chemical under the Chemical Substances Control Law and is also designated as a Class 1 Chemical Substance under the PRTR Law. This substance is used as a raw material for carboxymethyl cellulose, which is itself used as a thickening agent and product quality stabilizer in a wide variety of fields such as foodstuffs, civil engineering, and building materials. In addition, the substance is used as a raw material for herbicides, surfactants, and perm solutions. The production and import quantity in fiscal 2022 was 17,423 t.

2.Exposure assessment

Total release to the environment in fiscal 2022 under the PRTR Law was approximately 0.22 t, and all releases were notified. Most of the notified releases were to the atmosphere. In addition, approximately 3.5 t was transferred to waste materials. The major source of notified releases was the chemical industry. A multi-media 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 to the atmosphere in particular, the predicted proportion distributed to water bodies would be 58.7%, and the predicted proportion distributed to soil would be 40.7%. Where the largest quantities were estimated to have been released to public water bodies, the predicted proportion distributed to water bodies would be 92.9%.

The maximum expected concentration of exposure to humans via inhalation could not be defined because ambient atmospheric and indoor air quality data could not be obtained. Further, the mean annual value for atmospheric concentration in fiscal 2022 was calculated by use of a plume-puff model on the basis of releases to the atmosphere notified under the PRTR Law for fiscal 2022: this model predicts a maximum level of 0.055 μg/m^3.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.033 μg/L for public freshwater bodies, and about 0.10 μg/L for seawater. When releases reported under the PRTR Law in fiscal 2022 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 0.011 μg/L. Further, when releases reported under the PRTR Law to public freshwater bodies estimated from the reported transfer to sewage in fiscal 2014, which was a year in which a notifications ran at a high level compared with other years, 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 0.0063 μg/L.

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3. Initial assessment of health risk

Since the quality standard of drinking water has already been established for this substance, the initial assessment did not cover the health risk via oral exposure.

This substance is corrosive to the eyes, the skin and the respiratory tract. Inhalation of this substance at high concentrations may cause lung edema after corrosive effects on the eyes and the upper respiratory tract have become manifest. When 5% or more of the skin surface is severely affected, life-threatening intoxication may occur. Exposure to this substance may cause death as well as effects on metabolism, metabolic acidosis and multiple organ failure. Since these effects may be delayed, medical observation is required.

Since not enough information was available on the carcinogenicity of the substance, the initial assessment was conducted based on information on its non-carcinogenic effects.

The 'non-toxic level' for inhalation exposure could not be identified.

Regarding inhalation exposure, due to the lack of identified 'non-toxic level' and exposure concentrations, the health risk could not be assessed. However, the tentative 'non-toxic level' for inhalation exposure could be derived from the conversion of the 'non-toxic level' for oral exposure, assuming that 100% of the inhaled substance is absorbed. The NOAEL of 3.5 mg/kg/day for oral exposure (based on significant decreases in the absolute and relative liver and the absolute kidney weights and significant increase in the relative testes weight), determined from toxicity tests in rats, was identified as the 'non-toxic level' for oral exposure, from which the tentative 'non-toxic level' for inhalation exposure of 12 mg/m^3 was obtained. The maximum concentration (annual mean) in ambient air near the operators that are releasing a large amount of the substance was estimated to be 0.055 μg/m^3 based on the releases into air reported in FY 2022 under the PRTR Law. The MOE for reference would be 22,000 which is calculated from the estimated maximum concentration (annual mean) in ambient air and the tentative 'non-toxic level' of 12 mg/m^3 and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Therefore, as a comprehensive judgment, the collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air.

Toxicity					Exposure assessment		Result of risk assessment		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'	(−) mg/kg/day	(−)	(−)	Drinking water	(−) μg/kg/day	MOE	(−)	(−)
					Groundwater	(−) μg/kg/day	MOE	(−)	
Inhalation	'Non-toxic level'	− mg/m^3	−	−	Ambient air	− μg/m^3	MOE	−	○
					Indoor air	− μg/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} of 33 μg/L for growth inhibition in the green alga *Desmodesmus subspicatus*, a 48-h EC_{50} of 74,200 μg/L for swimming inhibition in the crustacean *Daphnia magna*, a 96-h LC_{50} of 72,500 μg/L for the fish species *Oryzias latipes* (medaka), and a 14-d EC_{50} of 5800 μg/L for growth inhibition in the water-milfoil *Myriophyllum sibiricum*. Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 0.33 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 6 μg/L for growth inhibition in the green alga *D. subspicatus*, a 21-d NOEC of 32,000 μg/L for reproductive inhibition in the crustacean *D. magna*, a 35-d NOEC of less than 25,000 μg/L for mortality in the fish species *Danio rerio* (zebrafish embryos), and a 14-d NOEC of 2500 μg/L for growth inhibition in the water-milfoils *Myriophyllum spicatum* and *M. sibiricum*. Accordingly, based on these chronic toxicity values and an assessment factor of 10, a predicted no effect concentration (PNEC) of 0.6 μg/L was obtained.

The value of 0.33 μg/L obtained from the acute toxicity to the green alga was used as the PNEC for this substance.

The PEC/PNEC ratio is 0.1 for freshwater bodies and 0.3 for seawater. Accordingly, efforts to collect data for determining ecological risk are considered necessary.

When releases reported under the PRTR Law in fiscal 2022 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 0.011 μg/L, and the ratio of this value to PNEC is 0.03.

However, when taking into consideration assessment of ecological risk based on the PEC/PNEC ratio, based on a comprehensive review of the above findings efforts to collect further data are considered necessary. The same conclusion is reached even when considering the PNEC value based on chronic toxicity values.

Given that this substance appears to exhibit significant toxicity towards algae, further efforts to collect and carefully examine data are considered necessary for species exhibiting high sensitivity.

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)		
Green algae	Acute	EC_{50} Growth inhibition	100	0.33	Freshwater	0.033	0.1	▲
					Seawater	0.10	0.3	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Not covered by this assessment	(－)
	Inhalation exposure	No need for further work	○
Ecological risk	Requiring information collection.		▲

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