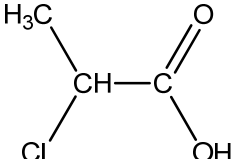| 4	CAS No: 598-78-7	Substance: 2-Chloropropionic acid

Chemical Substances Control Law Reference No.: 2-1157 (chloropropionic acid)

PRTR Law Cabinet Order: 1-122

Molecular Formula: $C_3H_5ClO_2$

Molecular Weight: 108.52

Structural Formula:

1. General information

This substance is freely miscible with water, the partition coefficient (1-octanol/water) (log K_{ow}) is less than -2.4 (pH = 7.2), and the vapor pressure is 3 mmHg (= 400 Pa) (60°C). Biodegradability (aerobic degradation) is judged to be good.

This substance is designated as a Class 1 Designated Chemical Substance under the Law Concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law). The main use of this substance is as an organic synthesis raw material (agricultural chemicals, pharmaceuticals), particularly for agricultural chemicals. The production and import quantity in fiscal 2012 was not disclosed because the number of reporting businesses was not more than two, but in fiscal 2011 it was less than 1,000 t. The production and import category under the PRTR Law is 1 to < 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2012 under the PRTR Law was 0 t. Because emissions based on the PRTR Law could not be obtained, predictions of proportions distributed to individual media were made by using a Mackay-type level III fugacity model. This indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to the soil and water bodies would be largest.

The maximum expected concentration of exposure to humans via inhalation, based on ambient air, was generally 0.0009 µg/m^3. The maximum expected oral exposure was estimated to be generally less than 0.00024 µg/kg/day on the basis of calculations from data for public freshwater bodies. However, because emissions to freshwater bodies based on the PRTR Law were 0 t in fiscal 2012, releases to public freshwater bodies in fiscal 2011 reported according to the PRTR Law 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 0.00084 µg/L. Using this estimated concentration for rivers to calculate oral exposure gave 0.000034 µg/kg/day. The exposure level to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on basis of its physicochemical properties.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was reported to be generally less than 0.006 µg/L for public freshwater bodies and less than 0.006 µg/L for seawater. However, because emissions to freshwater bodies based on the PRTR Law were 0 t in fiscal 2012, releases public freshwater bodies in fiscal 2011 reported according to the PRTR Law 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 0.00084 µg/L.

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3. Initial assessment of health risk

The substance is corrosive to the eyes, skin and respiratory tract. Corrosion may also occur by ingestion. When inhaled, sore throat, coughing, burning sensation, breathing difficulty and shortness of breath may occur,

while abdominal pain, burning sensation, shock or collapse may occur when ingested. Contact of the substance with the skin and eyes may cause redness, pain and severe burns.

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

With regard to the oral exposure to the substance, the NOAEL of 8 mg/kg/day (based on hypersensitiveness), obtained for mid-term and long-term toxicity tests on rats, was divided by a factor of 10 due to their short test periods. The outcome of 0.8 mg/kg/day was considered to be the reliable lowest dose of the substance and was identified as its 'non-toxic level*'. As for the inhalation exposure to the substance, the 'non-toxic level*' could not be established.

Concerning the oral exposure to the substance, the predicted maximum exposure level was below 0.00024 µg/kg/day, assuming the ingestion of water from public water bodies and freshwater. The MOE (Margin of Exposure) of above 330,000 was derived from the substance's 'non-toxic level*' of 0.8 mg/kg/day and the predicted maximum exposure level, after the division by a factor of 10 to convert animal data to human data. In addition, the amount of emissions into the environment was 0 t according to FY 2012. The MOE of 2,400,000 was derived from the maximum exposure level of 0.000034 µg/kg/day; derived itself from the concentrations of the substance in effluents from the high discharging plants, calculated according to the reported emissions data in FY 2011 under the PRTR Law. As exposure to the substance in the environment through diet is limited, the MOE would not change significantly even when this exposure is included. Therefore, no further work would be required at present to assess the health risk assessment of this substance for the oral exposure.

Regarding the inhalation exposure to the substance, the 'non-toxic level*' could not be established, and no health risk assessment could be made. Nonetheless, assuming a 100 % absorption and converting the 'non-toxic level*' for oral exposure to the inhalation one, the 'non-toxic level*' would be 2.7 mg/m³. The MOE of 30,000 was derived from this level and the predicted maximum exposure concentration in ambient air of 0.0009 µg/m³, and after the division by a factor of 10 to convert animal data to human data. Therefore, no further work would be required for the health risk assessment of this substance on inhalation exposure.

Exposure Path	Toxicity				Exposure assessment		Result of risk assessment			Judgment
	Criteria for risk assessment		Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	'Non-toxic level*'	0.8 mg/kg/day	Rat	Hypersensitiveness	Drinking water	— µg/kg/day	MOE	—	×	○
					Freshwater	<0.00024 µg/kg/day	MOE	> 330,000	○	
Inhalation	'Non-toxic level*'	— mg/m³	—	—	Ambient air	0.0009 µg/m³	MOE	—	×	(○)
					Indoor air	— µg/m³	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 73,400 µg/L for growth inhibition in the green alga *Pseudokirchnerella subcapitata*, and a 48-h EC_{50} of 74,400 µg/L for swimming inhibition in the crustacean *Daphnia magna*. Accordingly, based on these acute toxicity values and an assessment factor of 1000, a predicted no effect concentration (PNEC) of 73 µg/L was obtained.

With regard to chronic toxicity, the following reliable data was obtained: a 72-h NOEC of 25,000 µg/L for growth inhibition in the green alga *P. subcapitata*. Accordingly, based on this chronic toxicity value and an

assessment factor of 100, a PNEC of 250 µg/L was obtained.

The value of 73 µg/L obtained from the acute toxicity to the alga was used as the PNEC for this substance.

The PEC/PNEC ratio is less than 0.00008 for both freshwater bodies and seawater. In addition, because emissions to freshwater bodies based on the PRTR Law were 0 t in fiscal 2012, releases to public freshwater bodies in fiscal 2011 reported according to the PRTR Law 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 0.00084 µg/L, resulting in a ratio to PNEC of less than 0.1. Accordingly, further work is considered unnecessary at this time.

Hazard Assessment（Basis for PNEC）			Assessment Coefficient	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)			
Green algae	Acute	EC_{50} growth inhibition	1,000	73	Freshwater	<0.006	<0.00008	○	○
					Seawater	<0.006	<0.00008		

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5. Conclusions

		Conclusions	Judgment
Health risk	Oral exposure	No need for further work at present.	○
	Inhalation exposure	Although risk to human health could not be confirmed, collection of further information would not be required.	（○）
Ecological risk		No need for further work at present.	○

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

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

（○）: Although risk to human health could not be confirmed, collection of further information would not be required.

（▲）: Further information collection would be required for risk characterization.