1	CAS No.: 106-92-3	Substance: 1-Allyloxy-2,3-epoxypropane

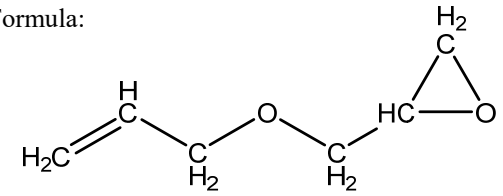
Chemical Substances Control Law Reference No.: 2-393

PRTR Law Cabinet Order No.: 1-29

Molecular Formula: $C_6H_{10}O_2$

Molecular Weight: 114.14

Structural Formula:



1. General information

The aqueous solubility of this substance is 1.41×10^5 mg/L, the partition coefficient (1-octanol/water) (log K_{ow}) is 0.46, and the vapor pressure is 3.6 mmHg (= 480 Pa) (20°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 37% and bioaccumulation is thought to be low. In addition, hydrolysis in water is thought to be extremely slow.

This substance is classified as a Class 1 Designated Chemical Substance under the PRTR Law. The major use of this substance is as a raw material for silane coupling agents. The production and import quantity in fiscal 2017 was not disclosed because the number of reporting businesses was not more than two. The production and import quantity under the PRTR Law was more than 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2017 under the PRTR Law was approximately 0.90 t, of which approximately 0.43 t or 48% was reported. All reported releases were to the atmosphere and approximately 50 t was transferred to waste material. The chemical industry was the sole source of reported releases. The largest releases to the environment including unreported releases were to soil. A multimedia model used to predict the proportions distributed to individual media in the environment indicates that in regions where the largest quantities were estimated to have been released to the environment overall or the atmosphere in particular, the predicted proportion distributed to water bodies was 78.0% and that to soil was 16.3%. Where the largest quantities were estimated to have been released to soil, the predicted proportion distributed to water bodies was 53.9% and that to soil was 45.5%.

The maximum expected concentration of exposure to humans via inhalation, based on general environmental atmospheric data, was around 0.012 μg/m^3. The mean annual value for the atmospheric concentration in fiscal 2017 was calculated by use of a plume-puff model on the basis of releases to the atmosphere reported under the PRTR Law; this model predicts a maximum level of 0.16 μg/m^3.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. However, past data measured for ground water and public freshwater bodies indicated a maximum expected exposure of around less than 0.008 μg/kg/day. Further, no releases to public freshwater bodies were reported in fiscal 2017 under the PRTR Law; accordingly, this substance's concentration in public water bodies is thought to be low. 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.

Data for setting the predicted environmental concentration (PEC) could not be obtained for this substance. Past data for public freshwater bodies and seawater indicated a value of around less than 0.2 μg/L. There were no releases to public water bodies reported in fiscal 2017 under the PRTR Law. On this account, public water body concentrations are thought to be low.

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3. Initial assessment of health risk

This substance is corrosive. Ingestion of the substance causes burning sensation, headache, dullness, drowsiness, nausea and vomiting. Inhalation causes cough, sore throat, burning sensation, drowsiness and lethargy, and may cause lung edema.

Contact with the skin causes dry skin, redness, pain and blisters. Contact with the eyes causes redness, pain, blurred vision and severe deep burns.

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 'non-toxic level' for oral exposure could not be identified. The NOAEL of 1 ppm for inhalation exposure (based on squamous metaplasia of the respiratory epithelium and the olfactory epithelium and chronic inflammation of the mucosa observed in the nasal passage), determined from medium-term toxicity tests in mice, was adjusted according to exposure conditions to obtain 0.18 ppm (0.84 mg/m^3), and subsequently divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.084 mg/m^3 was deemed to be the lowest reliable concentration and was identified as the 'non-toxic level' of the substance for inhalation exposure.

With regard to oral exposure, owing to the lack of identified 'non-toxic level' and exposure levels, the health risk could not be assessed. However, systemic effect (suppression of body weight gain) was observed, though not manifesting its statistical significance, in the 4 ppm or higher exposure groups in the study in mice, in addition to the local effects on respiratory tract specified as the endpoints to derive 'non-toxic level' for inhalation exposure. Considering this observation, the tentative 'non-toxic level' for oral exposure derived from the conversion of the 'non-toxic level' for inhalation exposure would be used to make conservative assessment of the health risk via oral exposure. Assuming that 100% of the ingested substance is absorbed, the tentative 'non-toxic level' for oral exposure would be 0.025 mg/kg/day. Assuming that the substance is absorbed via groundwater and public freshwater bodies, the maximum exposure level was estimated to be less than 0.008 μg/kg/day, based on past data on groundwater and public freshwater bodies reported in 2000. The MOE (Margin of Exposure) would exceed 310, when calculated from the estimated maximum exposure level and the converted 'non-toxic level', and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. 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 further information would not be required to assess the health risk of this substance via oral exposure.

With regard to inhalation exposure, the predicted maximum exposure concentration in ambient air was 0.012 μg/m^3, approximately. The MOE would be 700, when calculated from the maximum exposure concentration and the 'non-toxic level' of 0.084 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. This would lead to the health risk judgment that no further work would be required at present. However, the MOE for reference would be 53, when calculated from the concentration of 0.16 μg/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 the releases to air reported in FY 2017 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' - mg/kg/day	-	-	Drinking water	- μg/kg/day	MOE	-	○
				Groundwater	- μg/kg/day	MOE	-	
Inhalation	'Non-toxic level' 0.084 mg/m^3	Mice	Squamous metaplasia of the respiratory epithelium and the olfactory epithelium and chronic inflammation of the mucosa in the nasal passage	Ambient air	0.012 μg/m^3	MOE	700	▲
				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} exceeding 79,000 μg/L for growth inhibition in the alga *Raphidocelis subcapitata*, a 48-h EC_{50} of 50,000 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 30,000 μg/L for the fish species *Carassius auratus* (goldfish). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 300 μg/L was obtained.

With regard to chronic toxicity, the following reliable data was obtained: a 72-h NOEC of 20,000 μg/L for growth inhibition in the alga *R. subcapitata*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 200 μg/L was obtained.

The value of 200 μg/L obtained from the chronic toxicity to the alga was used as the PNEC for this substance.

Data for setting the predicted environmental concentration (PEC) could not be obtained for this substance. Accordingly, an assessment of ecological risk could not be made.

Past data for public freshwater bodies and seawater indicated a value of around less than 0.2 μg/L, and the ratio of this value with the PNEC is less than 0.001. There were no releases to public water bodies reported in fiscal 2017 according to the PRTR Law. On this account, public water body concentrations are thought to be low. Based on a comprehensive review of the above findings, there is little need to collect new data regarding this substance.

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	Chronic	NOEC Growth inhibition	100	200	Freshwater	—	—	○
					Seawater	—	—	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	Requiring information collection.	▲
Ecological risk	No need for further work.		○

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