9	CAS No.: 4170-30-3	Substance: Crotonaldehyde

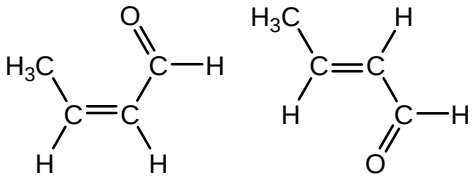
Chemical Substances Control Law Reference No.: 2-524

PRTR Law Cabinet Order No.:

Structural Formula:

Molecular Formula: C_4H_6O

Molecular Weight: 70.09



cis-form *trans*-form

1. General information

The aqueous solubility of this substance is 1.81×10^5 mg/1000g (20°C) and the partition coefficient (1-octanol / water) (log Kow) is 0.60(calculated value). The vapor pressure is 30.0 mmHg (= 4.0×10^3Pa) (20°C). Degradability (aerobic degradation) is considered to be sufficient. Generally, however, aldehydes are considered to be less hydrolyzable in the environment.

This substance (*trans*-form) is considered to be mainly used as a raw material for various chemicals and medicines such as butanol, crotonic acid, sorbinic acid, etc. The quantity of production in 2004 was approximately 16,000 tons (estimated value as crotonaldehyde *(trans*-form)).

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2. Exposure assessment

As this substance is not 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), release and transfer quantities could not be obtained. When predictions of distribution ratios by medium were made using the Mackay-Type Level III Fugacity Model, in the event of equal release to the atmosphere, water and soil, the distribution ratio was highest for soil and water.

Based on data for the ambient air, the predicted maximum exposure concentration for inhalation exposure to human beings was approximately 0.23 μg/m^3. The expected maximum concentration in the indoor air was 33.6μg/m^3. However, there is a report of the maximum concentration of 58.3μg/m^3 at the limited area. The predicted maximum oral exposure was estimated to be less than 0.08 μg/kg/day. The aqueous solubility of this substance is 1.81×10^5 mg/1000g and the bioconcentration is also predicted to be low, exposure from environmental media via the food chain is assumed to be low.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be less than 2 μg/L for both freshwater and seawater public water bodies.

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3. Initial assessment of health risk

This substance has a lachrymation property. Its vapor may result in severe irritation of the skin and respiratory tract, and causes corrosivity to the eyes. By ingestion, it may cause abdominal pains, burning sensation, diarrhea, nausea, vomiting. By ingestion, it may cause burning sensation, coughing, laboured breathing, shortness of breath, and sore throat. The inhalation of high concentration may cause lung edema and death. Contact to the skin and eyes may cause redness, burning sensation and pains, and redness, pain and severe burn, respectively.

There was insufficient information regarding the carcinogenicity of the substance. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

As the ‘Non-toxic level’ for oral exposure, the LOAEL of 2 mg/kg/day (altered hepatocellular foci) was obtained from the medium- and long-term toxicity testing for rats. As this was a LOAEL, it was divided by 10 to derived a value of 0.2 mg/kg/day as the ‘Non-toxic level’. As the ‘Non-toxic level’ for inhalation, the LOAEL of 8.6 mg/m^3 (lesion of nasal cavity) was obtained

from the medium- and long-term toxicity testing for rats. This value was adjusted to 1.5 mg/m^3 taking into the exposure situation. As this value was LOAEL, it was further divided by 10, and a value of 0.15 mg/m^3 was derived as the 'Non-toxic level'.

With regard to oral exposure, the predicted maximum exposure was approximately less than 0.08 μg/kg/day in case of the freshwater public water bodies groundwater intake. The MOE of 250 was derived from the 'Non-toxic level' of 0.2 mg/kg/day divided by the predicted maximum dose, and divided by 10, because the 'Non-toxic level' was established by means of animal testing. As the exposure to this substance through food intakes is estimated minor, even when the exposures through freshwater and food are combined, it would not greatly affect the MOE values. Accordingly, further action for assessment of its health risk from oral exposure to this substance would not be required at present.

For the inhalation, when the concentration in the ambient air was considered, the predicted maximum exposure concentration was approximately 0.23 μg/m^3. Accordingly, from the non-toxicity level of 0.15mg/m^3 and the predicted maximum inhalation concentration, the MOE of 65 was determined in the same way. For the concentration in the indoor air, the predicted maximum exposure concentration was 34 μg/m^3, and the MOE was 0.44. Accordingly, it would be required to collect information on inhalation exposure to this substance in the ambient air for its health risk assessment. On the other hand, for the health risk caused by the inhalation in the indoor air, this substance is considered to be a candidate of assessment in detail.

Information of toxicity				Exposure assessment		Result of risk assessment			Judgment
Exposure path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
oral	'Non toxic level' 0.2 mg/kg/day	Rats	Altered hepatocellular foci	Drinking water	– μg/kg/day	MOE	–	×	○
				Freshwater	< 0.08 μg/kg/day	MOE	> 250	○	
Inhalation	'Non toxic level' 0.15 mg/m^3	Rats	Lesion of nasal cavity	Ambient air	0.23 μg/m^3	MOE	65	▲	▲
				Indoor air	34 μg/m^3	MOE	0.44	■	■

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4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 72-hour EC_{50} growth inhibition value of 939 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 48-hour EC_{50} immobilization value of 995 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC_{50} value of 72 μg/L was found for the fish *Oryzias latipes* (medaka). Accordingly, an assessment factor of 100 was used, a predicted no effect concentration (PNEC) of 0.72 μg/L was obtained based on the acute toxicity values. With regard to chronic toxicity, reliable information of a 72-hour no observed effect concentration (NOEC) growth inhibition value of 42 μg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 20 μg/L was found for the crustacea *D. magna*. So an assessment factor of 100 was used, and a PNEC value that 0.20 μg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 0.20 μg/L obtained from the chronic toxicity for the crustacea was used.

The PEC/PNEC ratio was below 10 in both freshwater and seawater bodies. Therefore, at this point, the risk assessment could not be carried out. Because the PNEC value of this substance was small as 0.20 μg/L, it is considered to need for the effort to collect the information about the quantities of production and import, and the amount of release to the environment. The investigation of monitoring the environmental concentration is also required. It is also considered that the chronic toxicity testing in the fish is also required.

Hazard assessment (basis for PNEC)			Assessment factor	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Result of assessment
Species	Acute / chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacea (water flea)	Chronic	NOEC reproduction	100	0.20	Freshwater	< 2	< 10	×
					Seawater	< 2	< 10	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need of further work.	○
	Inhalation exposure	For the ambient air, there is thought to need for collection of information, and this substance is considered to be a candidate of assessment in detail.	▲ | ■
Ecological risk	Impossible of risk characterization. There is thought to be need to seek understanding the information of production, imported amounts and release to the environment, and to examine the implementation of measures, etc. of environmental concentration. In addition, there is thought to be need to examine the implementation of chronic toxicity tests in the fish.		×

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

Non-toxic level *

・When a LOAEL is available, it is divided by 10 to obtain a level equivalent to NOAEL.

・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.