3	CAS No.: 105-67-9	Substance: 2,4-Xylenol

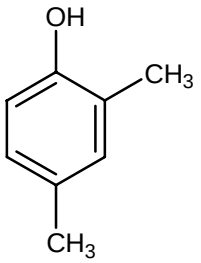
Chemical Substances Control Law Reference No.: 3-521(as dialkylene [C=1-5] phenol, and 4-57 (poly [1-3] alkyl [C=1-3] poly [1-3] hydroxypoly [1~5] phenyl)

PRTR Law Cabinet Order No.: 2-17

Molecular Formula: $C_8H_{10}O$

Molecular Weight: 122.17

Structural Formula:



1. General information

The aqueous solubility of this substance is 7.87 x 10^3 mg/l (25℃) and the partition coefficient (1-octanol / water) (log Kow) is 2.30. The vapor pressure is 0.0988 mmHg (- 13.2 Pa) (25°C, extrapolated value). Degradability (aerobic degradation) is considered not to be persistent, but this substance does not have hydrolizable groups.

This substance is a Class 2 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). It is used primarily as an agricultural chemical (pesticide), a precursor of medicine and an organic color. Production (shipment) and import quantities in 2001 were 100~below 1,000 tons (as xylenol), and export and import quantities in 2004 were 970 tons and 563 tons, respectively (each value was the total of xylenol and its salt form).

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2. Exposure assessment

As 2,4-Xylenol 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.

No predicted maximum exposure concentration for inhalation exposure to human beings could be established. However, it has been reported that when the data for a limited area (Kawasaki City) was used, it was less than 0.0023 μg/m^3. The predicted maximum oral exposure was estimated to be 0.018 μg/kg/day.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be 0.45 μg/L for freshwater and generally less than 0.005 μg/L for seawater public water bodies.

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3. Initial assessment of health risk

The effects of this substance are similar to those of phenol: it is corrosive to the skin, respiratory tract and eyes, and has corrosivity even by ingestion. Inhalation of an aerosol of this substance may cause lung oedema. Contact with skin or eyesmay cause redness, pain and burn. On ingestion it may cause burning sensation, abdominal pains, nausea, vomiting and shock/collapse. Inhalation may cause burning sensation, coughing, sore throat ,shortness of breath, etc.

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 the oral exposure, the NOAEL of 30mg/kg/day (increase in relative weight of kidney) was

obtained from the medium-and long-term toxicity testing for rats. This value was divided by 10 because of the short experimental period, and a value of 3 mg/kg/day was derived as the 'Non-toxic level'. For inhalation exposure, the 'Non-toxic level' was not estimated.

With regard to oral exposure, in case of intakes of freshwater public water bodies, the predicted maximum exposure was approximately 0.018 μg/kg/day. The MOE of 17,000 was derived from the 'Non-toxic level' of 3 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. The exposure to this substance through food intakes has not been estimated. However, considering the physical/chemical properties, presence of this substance and 2,6-xylenol in the freshwater public water bodies, and presence of 2,6-xylenol in foods, 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, because its 'Non-toxic level' was not determined, and the exposure concentrations have not been estimated, its health risk can not be identified. Released amount of this substance to the environment has not surveyed. Its half-life was estimated to be 0.90-9.0 hrs in the atmosphere. Considering the total release of 2,6-xylenol to the environment, there would be low necessity of collecting information on inhalation exposure to this substance in the ambient air for its health risk assessment.

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' 3 mg/kg/day	Rats	Increase in relative weight of kidney	Drinking water	– μg/kg/day		MOE	–	×	○
				Freshwater	0.018 μg/kg/day		MOE	17,000	○	
Inhalation	'Non toxic level' – mg/m^3	–	–	Ambient air	– μg/m^3		MOE	–	×	×
				Indoor air	– μg/m^3		MOE	–	×	×

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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 9,650 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 48-hour LC_{50} value of 2,100 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC_{50} value of 16,200 μg/L was found for the fish *Oryzias latipes* (medaka), a 60-hour IGC_{50} growth inhibitory concentration of 130,510μg/L for the other organism *Tetrahymena pyriformis* (*tetrahymena*). Accordingly, an assessment factor of 100 was used, a predicted no effect concentration (PNEC) 21 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 1,820 μg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 270 μg/L was found for the crustacea *D. magna*, and a 30-day NOEC growth inhibition value after hatching of 1,500μg/L for the fish *Pimephales promelas* (Fathead minnow), and a 2-day NOEC reproduction value of 2,000μg/L for the other organism *Brachionus calyciflorus* (Rotifer). So an assessment factor of 10 was used, and a PNEC value of 27 μg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 21 μg/L obtained from the acute toxicity for the crustacea was used.

The PEC/PNEC ratio was 0.02 for freshwater bodies and less than 0.0002 for seawater bodies. Accordingly, further work is thought to be unnecessary at this time.

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)	Acute	LC_{50} Mortality	100	21	Freshwater	0.45	0.02	○
					Seawater	< 0.005	< 0.0002	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need of further work.	○
	Inhalation exposure	Impossible of risk characterization. However, there is thought to be comparatively little need to collect information, etc.	×
Ecological risk	No need of further work.		○

［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.