4	CAS No.: 576-26-1	Substance: 2,6-Xylenol

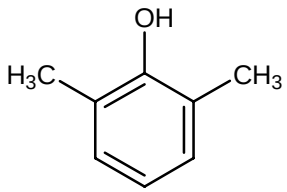
Chemical Substances Control Law Reference No.: 3-521(as dialkylene [C=1-5] phenol, and 4-57 (poly [1-3] alkyl [C=1-3] poly [1-3] hydroxypoly [1~5] phenyl)

PRTR Law Cabinet Order No.: 1-62

Molecular Formula: $C_8H_{10}O$

Molecular Weight: 122.17

Structural Formula:



1. General information

The aqueous solubility of this substance is 6.05 x 10^3 mg/l (25℃), and the partition coefficient (1-octanol / water) (log Kow) is 2.33. The vapor pressure is 0.253 mmHg (- 33.7 Pa) (25°C, extrapolated value). Degradability (aerobic degradation) is considered to be persistent, and this substance does not have hydrolizable groups in the environment.

This substance is a Type 3 Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances and 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). It is used primarily as a material of resin (PPE etc.), antioxidant, and anti-mold. 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

Total release to the environment in FY2004 under the PRTR Law came to 1.1 tons, all of which was reported. Release to the atmosphere accounted for a large part of the reported release. The main origins of release of the reported quantity to the atmosphere and public water bodies were only chemical industries.

The distributions into each environmental medium as determined by means of a multimedia model were 89.1% for soil and 5.4% for water bodies in the case of the region where the release quantity to the environment and atmosphere was considered to be the maximum. In the case of the region where the release quantity to the public water bodies was considered to be the maximum, the distributions were 74.6% for water bodies, and 16.4% for bottom.

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 0.0013 μg/m^3. The predicted maximum oral exposure was estimated to be 0.0437 μg/kg/day.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be approximately 0.093 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 and eyes, and has corrosivity even after ingestion.It may cause irritation of the respiratory tract, resulting in coughing, dizziness and headache. By ingestion it may cause burning sensation, abdominal pains, nausea, vomiting, diarrhea, dizziness and shock/collapse. Contact with skin or eyes may cause redness and burn.

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 0.6mg/kg/day (effects on body weight, blood pressure, SH

groups of blood serum and the internal organs, liver, kidney and spleen) 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 0.06 mg/kg/day was derived as the 'Non-toxic level'. For inhalation exposure, the 'Non-toxic level' could not be estimated.

With regard to oral exposure, in case of intakes freshwater from the public water bodies and food, the predicted maximum exposure was approximately 0.044 μg/kg/day. The MOE of 140 was derived from the 'Non-toxic level' of 0.06 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. 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. The total release of this substance to the environment was 1.1 tons, and most of the quantity of this substance was released to the atmosphere. Its half-life in the atmosphere was estimated to be 0.97-9.7 hrs, and the estimation of the distribution into each environmental medium suggested that this substance is scarcely distributed into atmosphere. Accordingly, 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	No observed adverse effect level 0.06 mg/kg/day	Rats	Effects on body weight, blood pressure, SH groups of serum and the internal organs, liver, kidney and spleen	Drinking water, Food	– μg/kg/day	MOE	–	×	○
				Freshwater, Food	0.044 μg/kg/day	MOE	140	○	
Inhalation	No observed adverse effect level – mg/m^3	–	–	Ambient air	– $\mu g/m^3$	MOE	–	×	×
				Indoor air	– $\mu g/m^3$	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 of 47,700 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 48-hour EC_{50} immobilization value of 11,100 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC_{50} value of 15,400 μg/L was found for the fish *Oryzias latipes* (medaka). Accordingly, an assessment factor of 100 was used, a predicted no effect concentration (PNEC) 110 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 3,940 μg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 538 μg/L was found for the crustacea *D. magna*. So an assessment factor of 100 was used, and a PNEC value of 5.4 μg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 5.4 μg/L obtained from the chronic toxicity for the crustacea was used.

The PEC/PNEC ratio was 0.02 for freshwater bodies and less than 0.0009 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)	Chronic	NOEC reproduction inhibition	100	5.4	Freshwater	0.093	0.02	○
					Seawater	< 0.005	< 0.0009	

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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.