20	CAS No.: 131-17-9	Substance: Diallyl phthalate

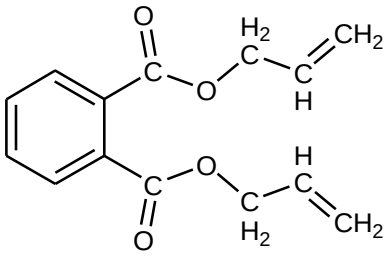
Chemical Substances Control Law Reference No.: 3-1325 (Diallyl phthalate)

PRTR Law Cabinet Order No.: － (Cabinet Order No. after revision*: 1-352)

Structural Formula:

Molecular Formula: $C_{14}H_{14}O_4$

Molecular Weight: 246.26



*Note: No. according to revised order enacted on October 1, 2009.

1. General information

The aqueous solubility of this substance is 182 mg/L (20°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 3.23, and the vapor pressure is 1.60×10^{-4} mmHg (=0.0213 Pa) (25°C). Biodegradability (aerobic degradation) is thought to be good. Its half-life for hydrolysis is more than 1 year (25°C, pH=4, 7) and 217-h (25°C, pH=9).

Based on a revision of substances regulated by the Law Concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law) (enacted on October 1, 2009), this substance was newly designated as a Class 1 Designated Chemical Substance. It is primarily used in crosslinking agents and reactive plasticizers. The production quantity of this substance as reported by the OECD is 1,000 to <10,000 t.

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2. Exposure assessment

Because this substance was not classified as a Class 1 Designated Chemical Substance prior to revision of substances regulated by the PRTR Law, release and transfer quantities could not be obtained. Predictions of distribution by medium using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportions distributed to soil and water bodies would be higher.

Data for setting the predicted maximum exposure to humans via inhalation could not be obtained. The predicted maximum exposure for indoor air was less than around 0.0050 μg/m^3 based on data from a limited area (Tokyo Metropolis). The predicted maximum oral exposure was estimated to be less than around 0.0004 μg/kg/day based on calculations from data for groundwater. The risk of exposure to this substance by intake from an environmental medium via food is considered slight.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was less than around 0.01 μg/L for both public freshwater bodies and seawater.

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3. Initial assessment of health risk

This substance may cause chemical pneumonia if swallowed in its liquid form as it is absorbed into the lungs. Redness of the eyes is caused by contact with this substance. Laboratory rats that were orally administered with the substance exhibited diarrhea, decrease in activity, hunchback posture, hyperpnea, and watery secretion around the noses and mouths before being sacrificed.

Sufficient information could not be obtained on its carcinogenicity, and its initial assessment was conducted on the basis of data on its non-carcinogenic effects.

As for its oral exposure, its LOAEL of 50 mg/kg/day (for the degeneration of liver tissue) obtained from mid-term and long-term toxicity tests for rats was adjusted against exposure conditions to produce 36 mg/kg/day. Since this was

LOAEL, it was then divided by 10 to provide 3.6 mg/kg/day as its 'non-toxic level*'.

As for its oral exposure, the predicted maximum exposure was estimated to be less than around 0.0004 µg/kg/day, when intakes of groundwater were assumed. Its margin of exposure (MOE) would be more than 900,000 when calculated from its 'non-toxic level*' of 3.6 mg/kg/day and the predicted maximum exposure, and then divided by 10 due to the fact that 'non-toxic level*' was obtained from animal experiments. Since risk associated with exposure to this substance through food intakes from the environment is presumed to be minimal, this exposure will not increase MOE significantly, and no further action will be required at the moment to assess health risk from oral exposure to this substance.

As for inhalation exposure to this substance, its 'non-toxic level' could not be identified, and its exposure concentrations were yet to be obtained. Its health risk could not be assessed. The 'non-toxic level' for its oral exposure, if 100% absorption is assumed for it, turns to be the 'non-toxic level' of 12 mg/m^3 for its inhalation exposure. When combined with the predicted maximum concentration of less than 0.005 µg/m^3 in the ambient air, MOE will be more than 240,000. Its half-life in the atmosphere is 1.2 to 12 hrs. When released to the atmosphere, most of it is expected to go to media other than the ambient air, and collection of information on its inhalation exposure to assess health risk associated with its inhalation exposure in the ambient air would not be required.

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*' 3.6 mg/kg/day	Rats	Degeneration of the liver tissues	Drinking water	–	µg/kg/day	MOE	–	×	○
				Groundwater	< 0.0004	µg/kg/day	MOE	> 900,000	○	
Inhalation	'Non-toxic level*' – mg/m^3	–	–	Ambient air	–	µg/m^3	MOE	–	×	(○)
				Indoor air	–	µg/m^3	MOE	–	×	×

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 is available for the short-term exposure, 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 median effective concentration (EC_{50}) of 5,500 µg/L for growth inhibition in the green algae *Desmodesmus subspicatus*; a 48-h EC_{50} of 16,200 µg/L for swimming inhibition in the crustacean *Daphnia magna;* and a 96-hour median lethal concentration (LC_{50}) of 440 µg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 4.4 µg/L was obtained. With regard to chronic toxicity, the following reliable data were obtained: a 72-h no observed effect concentration (NOEC) of 2,380 µg/L was obtained for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, and a 21-d NOEC of 3,200 µg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 24 µg/L was obtained. The value of 4.4 µg/L obtained from the acute toxicity to the fish species was used as the PNEC for this substance.

The PEC/PNEC ratio was less than 0.002 for both freshwater bodies and seawater. 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)		
Fish (medaka)	Acute	LC_{50} Mortality	100	4.4	Freshwater	<0.01	<0.002	○
					Seawater	<0.01	<0.002	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	Though a risk characterization cannot be determined, there would be little necessity of collecting information.	(○)
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

(○) : Though a risk characterization cannot be determined, there would be little necessity of collecting information.

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