4 CAS No.: 1321-74-0 Substance: Divinylbenzene

[91-14-5 (o-Divinylbenzene),

108-57-6 (m- Divinylbenzene)]

Chemical Substances Control Law Reference No.: 3-14

PRTR Law Cabinet Order No.: 2-37 (Cabinet Order No. after revision*: 1-202)

Molecular Formula: $C_{10}H_{10}$ Molecular Weight: 130.18

Structural Formula:

$$\begin{array}{c} \mathsf{CH_2} \\ \parallel \\ \mathsf{CH} \\ \mathsf{CH} \\ \parallel \\ \mathsf{CH_2} \end{array}$$

o-Divinylbenzene m-Divinylbenzene p-Divinylbenzene

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

1. General information

The aqueous solubility of this substance is 53 mg/L (o-, m-, p-isomers; 25°C; calculated value), the partition coefficient (1-octanol/water) (log K_{ow}) is 3.8 (o-isomer, m-isomer, p-isomer; calculated value), and the vapor pressure is 0.66 mmHg (=88 Pa) (o-isomer; 25°C; calculated value), 0.579 mmHg (=77.2 Pa) (m-isomer; 25°C), and 0.53 mmHg (=71 Pa) (p-isomer; 25°C; calculated value). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and bioaccumulation is thought to be nonexistent or low (officially published name is m- (or p-) divinylbenzene). The substance does not have any hydrolyzable groups in the environment.

This substance was classified as 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). However, it was removed from the Class 2 Designated Chemical Substance list as a result of the revision of substances regulated by the PRTR Law (enacted on October 1, 2009) and was newly designated as a Class 1 Designated Chemical Substance. In addition, it is designated as a Type III Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances. It is primarily used as a cross-linking agent in ion exchange resins, synthetic rubbers, ion exchange membranes, and styrenic resins such as ABS resin, MBS resin, and unsaturated polyester resin. The production and import quantity in fiscal 2007 was 1,340 t.

2. Exposure assessment

Because this substance was not 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, then for all isomers (*o*-isomer, *m*- isomer, and *p*- isomer), the proportion distributed to soil would be greater.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was reported to be generally less than $0.002 \mu g/L$ for public freshwater bodies, and less than $0.002 \mu g/L$ for seawater.

3. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h median effective concentration (EC₅₀)

of 1,830 μ g/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*; a 48-h EC₅₀ of 870 μ g/L for swimming inhibition in the crustacean *Daphnia magna*; and a 96-h median lethal concentration (LC₅₀) of 4,160 μ g/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 18 μ g/L was obtained. With regard to chronic toxicity, the following reliable data were obtained: a 72-h no observed effect concentration (NOEC) of 906 μ g/L for growth inhibition in the green algae *P. subcapitata*, and a 21-d NOEC of 353 μ g/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 3.5 μ g/L was obtained. The value of 3.5 μ g/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was less than 0.0006 for both freshwater bodies and seawater. Accordingly, further work is thought to be unnecessary at this time.

	Hazard asse	essment (basis	for PNEC)		Predicted no	Exposu	ire assessment	icted PEC/ Result of assessment (µg/L) 002 <0.0006	
	Species	Acute/ chronic	Endpoint	Assessment factor	effect concentration PNEC (µg/L)		Predicted environmental concentration PEC (µg/L)		Result of assessment
	Crustacean (water flea)	Chronic	NOEC Reproductive inhibition	100	3.5	Freshwater	< 0.002	< 0.0006	- 0
						Seawater	< 0.002	< 0.0006	

4 Conclusions

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	Conclusions			
Ecological risk	No need for further work.		0	
[Risk judgments]	O: No need for further work	▲: Requiring information collection		
	■: Candidates for further work	×: Impossibility of risk characterization		
	(O) : Though a risk characterize	zation cannot be determined, there would be	little necessity	
	collecting information.			
	(A): Further information collection	tion would be required for risk characterization.		