CAS No.: 53-16-7 Substance: Estrone

Chemical Substances Control Law Reference No.: 9-2145 (1,3,5(10)-Estratrien-3-ol-17-one)

PRTR Law Cabinet Order No.:

Molecular Formula:  $C_{18}H_{22}O_2$ 

Molecular Weight: 270.37

Structural Formula:

## 1.General information

The aqueous solubility of this substance is  $1.30 \text{ mg/1,000 g } (25^{\circ}\text{C})$ , the partition coefficient (1-octanol/water) (log K<sub>ow</sub>) is 3.13, and the vapor pressure is  $<7.5\times10^{-6}$  mmHg (<0.001 Pa) ( $25^{\circ}\text{C}$ ). The biodegradability (aerobic degradation) is characterized by a CO<sub>2</sub> emission of approximately 37%. In addition, this substance does not possess any hydrolyzable groups and hydrolysis does not occur under ambient environmental conditions.

The main uses of this substance are pharmaceuticals (estrogen), and medicinal product additives (medicinal soaps, cosmetics). Further, production of pharmaceuticals (estrogen and progestogen) was valued at 5,684 million yen in fiscal 2018.

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## 2.Exposure assessment

Because this substance is not classified as a Class 1 Designated Chemical Substance under the PRTR Law, release and transfer quantities could not be obtained. Predictions of proportions distributed to individual media by use of a Mackay-type level III fugacity model indicate that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to soil would be largest.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was reported to be around 0.0077 µg/L for public water bodies and around 0.00025 µg/L for seawater. Further, a public freshwater body concentration of 0.0077 µg/L was detected downstream of a sewage treatment plant.

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## 3.Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC<sub>50</sub> exceeding 570 μg/L for growth inhibition in the alga *Raphidocelis subcapitata*, a 48-h LC<sub>50</sub> exceeding 1,000 μg/L for the marine copepod *Acartia tonsa*, a 96-h LC<sub>50</sub> exceeding 1,186 μg/L for the fish species *Danio rerio* (zebra fish), and a 48-h LC<sub>50</sub> exceeding 50,000 μg/L for the dugesiid triclad *Dugesia japonica*. However, a PNEC value could not be derived based on these acute toxicity values because they were all either obtained from limit tests or equivalent to limit tests.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 570  $\mu$ g/L for growth inhibition in the alga *R. subcapitata*, and a 21-d NOEC exceeding 100  $\mu$ g/L for reproductive inhibition in the crustacean *Tisbe battagliai*, and a 27-week NOEC of 0.047  $\mu$ g/L for reproductive inhibition in the fish species *Oryzias latipes* (medaka). Accordingly, based on this chronic toxicity value and an assessment factor of 10, a PNEC of 0.0047  $\mu$ g/L was obtained.

The value of 0.0047 μg/L obtained from the chronic toxicity to the fish species was used as the PNEC for this substance. The PEC/PNEC ratio is 1.6 for freshwater bodies and 0.05 for seawater; accordingly, this substance is a candidate for detailed assessment of ecological risk. A comprehensive review of the above findings draws the same conclusion.

Hazard	ard assessment (basis for PNEC)		Predict	Predicted no effect	Exposure assessment			
Species	Acute/ chronic	Endpoint	Assessment coefficient	concentration PNEC (µg/L)	Water body	Predicted environmental concentration PEC (µg/L)	PEC/ PNEC ratio	Comprehensive judgment
Fish	Chronic	NOEC Reproductive	10	0.0047	Freshwater	0.0077	1.6	•
Oryzias latipes	Cinome	inhibition		0.0047	Seawater	0.00025	0.05	_

## 4. Conclusions

	Conclusions	Judgment
Ecological risk	Candidates for further work.	

[Risk judgments] O: No need for further work

▲: Requiring information collection

■: Candidates for further work

×: Impossibility of risk characterization