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|---|---|---|
| 7 | CAS No.: 1321-74-0 [91-14-5 (*o*-Divinylbenzene), 108-57-6 (*m*-Divinylbenzene), 105-06-6 (*p*-Divinylbenzene)] | Substance: Divinylbenzene |

Chemical Substances Control Law Reference No.: 3-14

PRTR Law Cabinet Order No.: 1-202

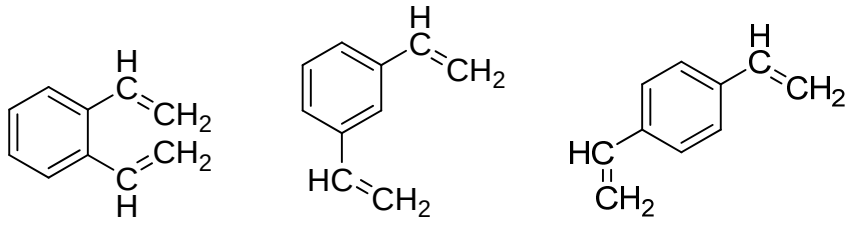
Molecular Formula:

$C_{10}H_{10}$

Molecular Weight:

130.19

Structural Formula:



*o*-Divinylbenzene *m*-Divinylbenzene *p*-Divinylbenzene

**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*-, *m*-, *p*-isomers, calculated value), and the vapor pressures are 0.66 mmHg (88 Pa) (*o*-isomer, 25°C, calculated value), 0.58 mmHg (77 Pa) (*m*-isomer, 25°C), and 0.60 mmHg (80 Pa) (*p*-isomer, 25°C, calculated value). Biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0% (average value). The toxicity of this substance is considered non-existent or low. The substance does not have any hydrolyzable groups under environmental conditions.

This substance is designated as 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). The main use of this substance is as a cross-linking agent for ion exchange resins and membranes, synthetic rubbers, styrenic resins such as ABS resin and MBS resin, and unsaturated polyester resins. The production and import quantity for fiscal 2012 and 2013 were not disclosed because the number of reporting businesses was not more than two. In fiscal 2011, the production and import quantity was 2,000 t. The production and import category under the PRTR Law is more than 100 t.

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**2. Exposure assessment**

Total release of divinylbenzene to the environment in fiscal 2013 under the PRTR Law was approximately 0.5 t, and all releases were reported. The major destination of reported releases was the atmosphere. In addition, approximately 3.3 t was transferred to waste materials. The sole source of reported releases was the chemical industry. A multi-media model used to predict the proportions distributed to individual media in the environment indicated that in regions where the largest quantities were estimated to have been released to the environment overall or public water bodies and the atmosphere in particular, the predicted proportion distributed to the atmosphere was 65.1%, and that distributed to water bodies was 19.3%.

The maximum expected concentration of exposure to humans via inhalation, based on general environmental atmospheric data, was around less than 0.013 μg/$m^3$. The mean annual value for the atmospheric concentration in fiscal 2013 was calculated by using a plume-puff model on the basis of releases to the atmosphere reported according to the PRTR Law; this model predicted a maximum level of 0.44 μg/$m^3$. The maximum expected oral exposure was estimated to be generally less than 0.00008 μg/kg/day on the basis of calculations from data for public freshwater bodies. The risk of exposure to this substance by intake from an environmental medium via food is considered slight, based on its low bioaccumulation.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was

reported to be generally less than 0.002 μg/L for public freshwater bodies and less than 0.002 μg/L for seawater.

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**3. Initial assessment of health risk**

The mixture of the isomers of this substance is irritating to the eyes, skin and respiratory tract. Inhalation exposure causes coughs and sore throat. Contact with skin causes redness, and contact with the eyes causes redness and pain.

As sufficient information on the carcinogenicity of the mixture of isomers was not available, the initial assessment was conducted on the basis of information on its non-carcinogenic effects.

The NOAEL of 30 mg/kg/day for oral exposure (based on relative liver weight gain), determined from medium-term and long-term toxicity tests in rats, was divided by a factor of 10 to account for extrapolation from sub-chronic to chronic exposure. The obtained value of 3.0 mg/kg/day was deemed to be the lowest reliable dose and was identified as the 'non-toxic level*' of the mixture for oral exposure.

The LOAEL of 10 ppm for inhalation exposure (based on respiratory epithelial metaplasia of olfactory glands and olfactory epithelium, atypical bronchiolar hyperplasia, etc.), determined from medium-term and long-term toxicity tests in mice, was adjusted for exposure conditions to obtain 1.8 ppm (9.6 mg/m$^3$), and subsequently divided by a factor of 10 to account for uncertainty in using LOAEL. The obtained value of 0.96 mg/m$^3$ was deemed to be the lowest reliable concentration and was identified as the 'non-toxic level*' of the mixture for inhalation exposure.

With regard to oral exposure, assuming the mixture is absorbed via public freshwater bodies, the predicted maximum exposure level was less than 0.00008 μg/kg/day, approximately. The MOE (margin of exposure) would be over 3,8000,000, when calculated from this value and the 'non-toxic level*'of 3.0 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Since exposure to the isomers in environmental media via food is presumed to be limited, its inclusion in the calculation would not change the MOE significantly. Therefore, no further work would be required at present to assess the health risk of the mixture via oral exposure.

With regard to inhalation exposure, the predicted maximum exposure concentration in ambient air was less than 0.013 μg/m$^3$, approximately. The MOE would be over 7,400, when calculated from this value and the 'non-toxic level*'of 0.96 mg/m$^3$, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans.

In addition, the maximum concentration (annual mean) in ambient air near the operators releasing large amount of the mixture to ambient air was estimated to be 0.44 μg/m$^3$ on the basis of the data reported in FY 2013 under the PRTR Law. The MOE would be 220, when calculated from the maximum concentration and the 'non-toxic level*'.

Therefore, no further work would be required at present to assess the health risk of the mixture via inhalation in ambient air.

| Toxicity | | | | Exposure assessment | | Result of risk assessment | | | Judgment |
|---|---|---|---|---|---|---|---|---|---|
| Exposure Path | Criteria for risk assessment | Animal | Criteria for diagnoses (endpoint) | Exposure medium | Predicted maximum exposure dose and concentration | | | | |
| Oral | 'Non-toxic level*' 3.0 mg/kg/day | Rat | relative weight increase of liver | Drinking Water | — μg/kg/day | MOE | — | × | ○ |
| | | | | Public freshwater bodies | <0.00008 μg/kg/day | MOE | >3,800,000 | ○ | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Inhalation | 'Non-toxic level*' 0.96 mg/m$^3$ | | Mouse | Respiratory epithelial metaplasia of olfactory glands and olfactory epithelium, atypical bronchiolar hyperplasia, etc. | Ambient air | <0.013 μg/m$^3$ | MOE | >7,400 | ○ | ○ |
| | | | | | Indoor air | — μg/m$^3$ | MOE | — | × | × |

Non-toxic level *

- When a LOAEL is available, it is divided by 10 to obtain a NOAEL-equivalent level.
- 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.

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**4. Initial assessment of ecological risk**

With regard to acute toxicity, the following reliable data were obtained: a 72-h $EC_{50}$ of 1,830 μg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, a 48-h of $EC_{50}$ 1,870 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h $LC_{50}$ of 4,160 μg/L in 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 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 906 μg/L for growth inhibition in the green algae *P. subcapitata*, and a 21-d NOEC of 353 μg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 3.5 μg/L was obtained.

The value of 3.5 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio is less than 0.0006 for both freshwater bodies and seawater; accordingly, further work is considered unnecessary at this time.

| Hazard Assessment (Basis for PNEC) | | | Assessment Coefficient | Predicted no effect concentration PNEC (μg/L) | Exposure Assessment | | PEC/PNEC ratio | Judgment based on PEC/PNEC ratio | Assessment result |
|---|---|---|---|---|---|---|---|---|---|
| Species | Acute/ chronic | Endpoint | | | Water body | Predicted environmental concentration PEC (μg/L) | | | |
| Crustacean *Daphnia magna* | Chronic | NOEC reproductive inhibition | 100 | 3.5 | Freshwater | <0.002 | <0.0006 | ○ | ○ |
| | | | | | Seawater | <0.002 | <0.0006 | | |

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**5. Conclusions**

| | Conclusions | | Judgment |
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| Health risk | Oral exposure | No need for further work at present. | ○ |
| | Inhalation exposure | No need for further work at present. | ○ |
| Ecological risk | No need for further work at present. | | ○ |

[Risk judgments] ○: No need for further work ▲: Requiring information collection
■: Candidates for further work ×: Impossibility of risk characterization
(○) : Although risk to human health could not be confirmed, collection of further information would not be required.
(▲) : Further information collection would be required for risk characterization.