| 2 | CAS No.: 97-00-7 | Substance: 1-Chloro-2,4-dinitrobenzene | | | | |
|--|---------------------------|---|--|--|--|--|
| Chemical | Substances Control Law Re | ference No.: 3-454 (Monochlorodinitrobenzene) | | | | |
| PRTR La | w Cabinet Order No.: | | | | | |
| Molecular Formula: C ₆ H ₃ ClN ₂ O ₄ | | Structural formula: | | | | |
| Molecula | r Weight: 202.55 | CI | | | | |
| | | O ₂ N NO ₂ | | | | |

1.General information

The aqueous solubility of this substance is 9.2 mg/1,000 g (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 2.17 (pH unknown), and the vapor pressure is 0.01 Pa at (20°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and the substance is not judged to be highly bioaccumulative. Further, this substance is believed to not hydrolyze under ambient environmental conditions because it does not possess any hydrolyzable groups.

The main uses of this substance are as a raw material for dyestuffs and pigments, and as a raw material for UV absorbers. The production and import quantity in fiscal 2021 as monochlorodinitrobenzene was less than 1,000 t.

2.Exposure assessment

This substance was classified as a Class 1 Designated Chemical Substance prior to revision of substances regulated by the PRTR Law. Total release to the environment in fiscal 2021 under the PRTR Law was 0 t. 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 maximum expected concentration of exposure to humans via inhalation could not be defined because ambient atmospheric and indoor air quality data could not be obtained. However, the concentration of this substance in the atmosphere is believed to be low given there were 0 kg of notified releases to the atmosphere in fiscal 2021 under the PRTR Law.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. However, a maximum expected exposure of around less than 0.0004 µg/kg/day was calculated based on past data measured for groundwater. In addition, public freshwater body concentrations originating from discharging business establishments are believed to be low given there were 0 kg of notified releases to in public freshwater bodies in fiscal 2021 under the PRTR Law. This substance is not judged to be highly bioaccumulative and as such, exposure from an environmental medium via ingestion is believed to be low.

Data to set the predicted environmental concentration (PEC) at a conservative value for water quality could not be obtained. However, albeit past data, a concentration of around less than 0.01 μ g/L was reported for public freshwater bodies and seawater.

Further, no releases to public freshwater bodies were notified in fiscal 2021 under the PRTR Law and as such, public freshwater body concentrations originating from discharging business establishments are believed to be low.

3. Initial assessment of health risk

This substance severely irritates the eyes and the skin. Inhalation of this substance will cause cyanosis, dizziness, headache, labored breathing, nausea, vomiting, and blurred vision. Ingestion will cause abdominal pain in addition to the same symptoms as inhalation. Contact with the skin will cause redness and pain. The substance can be absorbed into the body through the skin and may cause cyanosis, dizziness, etc. Contact with the eyes will cause redness and pain.

Since not enough information was available on the carcinogenicity of the substance, the initial assessment was conducted

based on information on its non-carcinogenic effects.

The NOAEL of 1 mg/kg/day for oral exposure (based on hyperplasia of squamous epithelium in forestomach), determined from toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.1 mg/kg/day was deemed the lowest reliable dose and was identified as the 'non-toxic level' of the substance for oral exposure. The 'non-toxic level' for inhalation exposure could not be identified.

Regarding oral exposure, due to the lack of identified exposure levels, the health risk could not be assessed. The predicted maximum exposure level was estimated to be approximately less than 0.0004 µg/kg/day, based on the past measurement data on groundwater in 2002. The MOE (Margin of Exposure) for reference would exceed 25,000 which is calculated from the estimated predicted maximum exposure level and the 'non-toxic level' of 0.1 mg/kg/day and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Since the release of this substance to public freshwater bodies was reported to be 0 kg in FY 2021 under the PRTR Law, the concentrations in public freshwater bodies derived from the discharging operators would not be high. In addition, exposure to the substance in environmental media via food is presumed to be limited, despite the lack of exposure level via food. Therefore, as a comprehensive judgment, the collection of further information would not be required to assess the health risk of this substance via oral exposure.

Regarding inhalation exposure, due to the lack of identified 'non-toxic level' and exposure concentrations, <u>the health risk</u> <u>could not be assessed</u>. Since the release of this substance to air was reported to be 0 kg in FY 2021 under the PRTR Law, the concentrations in ambient air would not be high. Therefore, <u>as a comprehensive judgment</u>, the collection of further information would not be required to assess the health risk of this substance via inhalation exposure.

| Toxicity | | | | Exposure assessment | | | | | | | |
|------------------|----------------|---------------|-------------------|---------------------|--------------------------------------|--------------------|-------------------|--|---------------------------------|---|---------------------------|
| Exposure Path | Criteria f | or risk | assessment | Animal | Criteria for diagnoses (endpoint) | Exposure medium | F maxin cor | Predicted num exposure lose and ncentration | Result of risk assessment | | Comprehensive judgment |
| Oral | 'Non- | 0.1 | | Data | Hyperplasia of | Drinking water | - | µg/kg/day | MOE | - | 0 |
| Oral | level*' | 0.1 mg/kg/day | Rats | forestomach/ | Groundwater | - | µg/kg/day | MOE | - | 0 | |
| Inhalation | 'Non- toxic | _ | mg/m ³ | - | _ | Ambient air | - | $\mu g/m^3$ | MOE | - | 0 |
| miniation | level*' | iiig/iii | | | 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.

4. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC₅₀ of 182 μ g/L for growth inhibition in the green alga *Raphidocelis subcapitat*a, a 48-h EC₅₀ of 655 μ g/L for swimming inhibition in the crustacean *Daphnia magna*, a 96-h LC₅₀ of 157 μ g/L for the fish *Oryzias latipes* (medaka), and a 24-h LC₅₀ of 1,300 μ g/L for the rotifer *Brachionus calyciflorus*. Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 1.5 μ g/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 5.96 μ g/L for growth inhibition in the green alga *R. subcapitata*, a 21-d NOEC of 183 μ g/L for reproductive inhibition on the crustacean *D. magna*, and a 38-d NOEC of 52 μ g/L for growth inhibition in the fish *O. latipes* (medaka). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a PNEC of 0.59 μ g/L was obtained.

The value of 0.59 μ g/L obtained from the chronic toxicity to the green alga was used as the PNEC for this substance.

Data for setting the predicted environmental concentration (PEC) could not be obtained for this substance. Accordingly, an assessment of ecological risk could not be made.

Further, while the data is more than 10 years prior, reports of a maximum PEC of less than 0.01 μ g/L for public freshwater bodies and seawater exist. The ratios of these concentrations to the predicted no effect concentration (PNEC) are less than 0.02.

Further, no releases to public freshwater bodies were notified in fiscal 2021 under the PRTR Law and as such, public freshwater body concentrations originating from discharging business establishments are believed to be low. Accordingly, <u>based on a comprehensive review of the above findings</u>, efforts to collect data are considered unnecessary at this time. In addition, at one point in time several years ago, releases were reported under the PRTR Law. Using this data to estimate river concentrations gave a value close to the PNEC. Accordingly, water quality surveys in the vicinities of discharge sources should be conducted if there is a possibility that environmental concentrations may increase in the future due to trends in manufacturing and import volumes.

| Hazard assessment (basis for PNEC) | | | | Predicted no effect | Expo | osure assessment | PD C/ | ~ | |
|------------------------------------|----------------|---------------------------|------------|------------------------------|------------|--|--------------------|---------------------------|--|
| Species | Acute/ chronic | Endpoint | Assessment | concentration PNEC (µg/L) | Water body | Predicted environmental concentration PEC (µg/L) | PEC/ PNEC ratio | Comprehensive judgment | |
| Green algae | Chronic | NOEC Growth inhibition | 10 | 0.59 | Freshwater | _ | _ | 0 | |
| | | | | | Seawater | _ | | Ŭ | |

5. Conclusions

| | | Conclusions | Judgment | |
|--------------------|---------------------------|---------------------------|----------|--|
| | Oral exposure | No need for further work. | 0 | |
| Health fisk | Inhalation exposure | No need for further work. | 0 | |
| Ecological risk | No need for further work. | | | |

[Risk judgments] O: No need for further work

■: Candidates for further work

▲: Requiring information collection

×: Impossibility of risk characterization