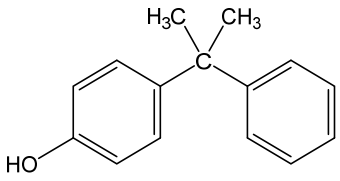
| 7 | CAS No： 599-64-4 | Substance: 4-(2-Phenylpropan-2-yl)phenol |
|---|---|---|

Chemical Substances Control Law Reference No.: 4-122 (4-(α,α-Dimethylbenzyl)phenol)
PRTR Law Cabinet Order No.:

Molecular Formula: $C_{15}H_{16}O$ Structural Formula:

Molecular Weight: 212.29




**1. General information**

The aqueous solubility of this substance is 18 mg/L (22°C, pH=5), the partition coefficient (1-octanol/water) (log $K_{ow}$) is 3.7 (23°·C) (pH=5.7), and the vapor pressure is 0.1 Pa (38°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0% (mean value), biodegradability is judged to be limited, and the substance is not judged to be highly bioaccumulative. In addition, this substance is stable towards hydrolysis (pH = 4, 7, 9; 50°C; 5 d).

The main uses of this substance are as a surfactant raw material, resin modifier (phenolic resin, epoxy resin, polycarbonate resin, etc.), a fungicide, an agricultural chemical intermediate, a plasticizer, and a stabilizer. The production and import category in fiscal 2019 was 1,000 t.

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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 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.

Data for potable water, groundwater, food, and soil to assess oral exposure could not be obtained. Assuming intake solely from public freshwater bodies, a maximum expected exposure of 0.0038 μg/kg/day is obtained. Further, albeit data for a limited area, calculations for public freshwater bodies gave a daily exposure of around 0.0064 μg/kg/day. The exposure to this substance by intake from an environmental medium via food is considered slight as it is judged not to be highly bioaccumulative.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms was around 0.094 μg/L for public freshwater bodies and around 0.0099 μg/L for seawater. Further, albeit based on data for a limited area, a maximum value of around 0.16 μg/L has been reported for public freshwater bodies.

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**3. Initial assessment of health risk**

No information was available on acute symptoms in humans caused by this substance. Although the rats exposed to an oral dose of this substance displayed diarrhea and soiled fur surrounding the anus and the urinary meatus, there were no abnormal findings in the autopsy.

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 5 mg/kg/day for oral exposure (based on suppression of body weight gain, the increased relative weight of the testis, the decreased relative weight of the spleen, etc.), determined from toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.5 mg/kg/day was deemed to be 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, assuming that the substance is absorbed via public freshwater bodies, the predicted maximum

exposure level would be 0.0038 μg/kg/day, approximately. The MOE (Margin of Exposure) would be 13,000 which is calculated from the predicted maximum exposure level and the 'non-toxic level' of 0.5 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. This would lead to the health risk judgment that no further work would be required at present. In addition, the MOE would be 7,800 which is calculated from the estimated maximum exposure level of 0.0064 μg/kg/day, approximately, according to the data in a certain area on public freshwater bodies. Since exposure to the substance in environmental media via food is presumed to be limited despite the lack of exposure level via food, including it in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, no further work would be required at present 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, the health risk could not be assessed. The vapor pressure of the substance is low, and predictions of the multimedia fugacity model indicated that the proportion distributed to air was very little. Therefore, as a comprehensive judgment, the collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air.

| Toxicity | | | | Exposure assessment | | MOE | | Comprehensive judgment |
|---|---|---|---|---|---|---|---|---|
| Exposure Path | Criteria for risk assessment | Animal | Criteria for diagnoses (endpoint) | Exposure medium | Predicted maximum exposure dose and concentration | | | |
| Oral | 'Non-toxic level' 0.5 mg/kg/day | Rats | Suppression of body weight gain, the increased relative weight of the testis, the decreased relative weight of the spleen, etc. | Drinking water | - μg/kg/day | MOE | - | ○ |
| | | | | Public freshwater bodies | 0.0038 μg/kg/day | MOE | 13,000 | |
| 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 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 1,390 μg/L for growth inhibition in the green alga species *Raphidocelis subcapitata*, a 48-h $EC_{50}$ 900 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h $LC_{50}$ of 900 μg/L for the fish species *Oncorhynchus mykiss* (rainbow trout). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 9 μg/L was obtained.

With regard to chronic toxicity, the following reliable datum was obtained: a 72-h NOEC of 330 μg/L for growth inhibition in the green alga species *R. subcapitata*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a predicted no effect concentration (PNEC) of 3.3 μg/L was obtained.

The value of 3.3 μg/L obtained from the chronic toxicity to the green alga was used as the PNEC for this substance.

The PEC/PNEC ratio is 0.03 for freshwater bodies and less than 0.003 for seawater. Further work to assess the ecological risk this substance is considered unnecessary at this time

A maximum value of around 0.16 μg/L has been reported for public water bodies, albeit for a limited area. The ratio of this value to PNEC is 0.05.

According, based on a comprehensive review of the above findings, there is little need to collect new data regarding this substance.

| Hazard assessment (basis for PNEC) | | | Assessment coefficient | Predicted no effect concentration PNEC (μg/L) | Exposure assessment | | PEC/ PNEC ratio | Comprehensive judgment |
|---|---|---|---|---|---|---|---|---|
| Species | Acute/ chronic | Endpoint | | | Water body | Predicted environmental concentration PEC (μg/L) | | |
| Green algae | Chronic | NOEC Growth inhibition | 100 | 3.3 | Freshwater | 0.094 | 0.03 | ○ |
| | | | | | Seawater | 0.0099 | 0.003 | |

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**5. Conclusions**

| | Conclusions | | Judgment |
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| Health risk | Oral exposure | No need for further work | ○ |
| | Inhalation exposure | No need for further work | ○ |
| 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