4 CAS No.: 6165-51-1 Substance: 1,4-Dimethyl-2-(1-phenylethyl) benzene

Chemical Substances Control Law Reference No.: 4-38 (1-Phenyl-1-xylyl ethane) and 4-244 (α-Methylbenzyl xylene)

PRTR Law Cabinet Order No.:

Molecular Formula: C_{16}H_{18} Structural formula:

![Structural formula](image)

1. General information

   The aqueous solubility of this substance is 0.96 mg/L (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 5.39 (25°C), and the vapor pressure is 1.6×10^{-4} mmHg (=0.021 Pa) (25°C). Biodegradation (aerobic degradation) is difficult, and bioaccumulation is thought to be nonexistent. The substance is stable with respect to hydrolysis (pH=4, 7, 9; 50°C; 5 days).

   This substance is designated as a Type II and Type III Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances. The main use is as a substitute solvent for PCB, with approximately 60% being used as a solvent in pressure sensitive paper dyestuffs and approximately 40% used in industrial condenser oil. Small quantities are used as epoxy resin and urethane resin plasticizers and as a substitute solvent for trichloroethane. The production (shipments) and import quantity in fiscal 2009 was 351 t.

2. Exposure assessment

   Because this substance is not classified 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), 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, the proportions distributed to soil would be greater.

   The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was generally 0.017 µg/L for public freshwater bodies and generally less than 0.0021 µg/L for seawater.

3. Initial assessment of ecological risk

   With regard to acute toxicity, the following reliable data were obtained: a 48-h EC_{50} of 250 µg/L for swimming inhibition in the crustacean *Daphnia magna* and a 96-h LC_{50} of 310 µg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment coefficient of 100, a predicted no effect concentration (PNEC) of 2.5 µg/L was obtained.

   With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 370 µg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, a 21-d NOEC of 9 µg/L for reproductive inhibition in the crustacean *D. magna*, and a 40-d NOEC of 33.8 µg/L for growth inhibition and post-hatching mortality in the fish species *O. latipes* (killifish). Accordingly, based on this chronic toxicity value and an assessment coefficient of 10, a predicted no effect concentration (PNEC) of 0.9 µg/L was obtained. The value of 0.9 µg/L obtained from the chronic
toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.02 for freshwater bodies and less than 0.002 for seawater. Accordingly, further work is thought to be unnecessary at this time.

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<td>Daphnia magna</td>
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<td>NOEC reproductive inhibition</td>
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### 4. Conclusions

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<td>Ecological risk</td>
<td>No need of further work at present</td>
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[Risk judgments] ○: No need for further work  ▲: Requiring information collection
■: Candidates for further work  ×: Impossibility of risk characterization
（○）: Though a risk characterization cannot be determined, there would be little necessity of collecting information.
（▲）: Further information collection would be required for risk characterization.