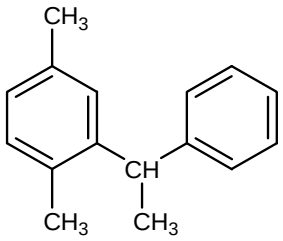
5	CAS No.: 6165-51-1	Substance: 1,4-Dimethyl-2-(1-phenylethyl) benzene

Chemical Substances Control Law Reference No.:4-38 (1-phenyl-1-xylylethane) and 4-244 (α-methylbenzylxylene)
PRTR Law Cabinet Order No.:
Molecular Formula: $C_{16}H_{18}$
Molecular Weight: 210.31

Structural formula:



1. General information

The water 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 (=0.021Pa) (25°C). This substance is judged not to be readily biodegradable (aerobic degradation), and not to be bioaccumulative. Furthermore, the substance does not hydrolyze (pH=4, 7, 9, 50°C, 5 days).

The main use is as a substitute solvent for PCBs, with approximately 60% used as a solvent for pressure sensitive paper dye, and approximately 40% used in industrial condenser oils. In addition, a small quantity is used as a plasticizer for epoxy resin and urethane resin, and as a replacement solvent for trichloroethane. The production and import quantity in FY 2009 was 351 t.

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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 proportion distributed to soil would be greater.

Data for setting the predicted maximum exposure to humans via inhalation could not be obtained. The predicted maximum oral exposure was estimated to be around 0.00068 μg/kg/day based on 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 estimates of oral exposure using estimated concentrations in fish.

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

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3. Initial assessment of health risk

There was no information available on acute toxicity of this substance to humans. In an acute toxicity test, where rats were treated with a single gavage administration of the substance, one female rat died on the first day after its administration and one male and one female rats died on the second day after its administration, among those administered 2,000 mg/kg/day of five males and five females. Reduced body weight and suppressed body weight increase were observed for rats administered the substance at no less than 1,000 mg/kg/day. For those administered the substance at 2,000 mg/kg/day, effects on general health condition, such as reduction in locomotor activity, bradypnea and side position, and on kidney, such as granular cast and protein cast, were observed.

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

As for oral exposure to the substance, a LOAEL of 12.5 mg/kg/day (for reduction of adrenal gland weight and the

atrophy of zona fasciculata cells) was obtained from mid- and long-term toxicity tests on rats. It was then divided by 10 as is always the case with LOAEL and was further divided by 10 due to their short test periods. 0.13 mg/kg/day was deemed to be the lowest reliable dose without any effect, and this was identified as its 'non-toxic level*'. As for inhalation exposure, its 'non-toxic level*' could not be identified.

As for its oral exposure, its mean exposure would be about 0.00011 μg/kg/day and its predicted maximum exposure would be around 0.00068 μg/kg/day, respectively, if its intakes through freshwater from public water bodies were assumed. The MOE would be 19,000 when calculated from the 'non-toxic level*' of 0.13 mg/kg/day and the predicted maximum exposure, and divided by 10 for conversion of the 'non-toxic level*' from animal experiments to an equivalent dose for humans. Since exposure to this substance through food intakes in the environment be limited, significant changes in the MOE would not be likely, even when this exposure were combined. Therefore, further actions would not be required at the moment to assess health risk from oral exposure to this substance.

As for inhalation exposure to the substance, lack of available information on its 'non-toxic levels*' and exposure concentrations did not allow its health risk assessment. The half life of the substance in the ambient air is estimated to be 2.9 to 29 hours, and when emitted to the ambient air, it rarely remains there. Therefore, collection of information would not be required to assess health risk from inhalation exposure to this substance in the 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 * ' 0.13 mg/kg/day	Rats	Reduced adrenal gland weight, atrophy of zona fasciculata cells	Drinking water	—	μg/kg/day	MOE	—	×	○
				Freshwater	0.00068	μg/kg/day	MOE	19,000	○	
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 level equivalent to NOAEL.

・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 48-h EC_{50} of 250 μg/L for immobilization in the crustacean *Daphnia magna*; and a 96-h LC_{50} of 310 μg/L for the fish (medaka) *Oryzias latipes*. Accordingly, based on these acute toxicity values and an assessment factor 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 the 9 μg/L for reproductive inhibition in 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* (medaka). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a predicted no effect concentration (PNEC) of 0.9 μg/L was obtained. This 0.9 μg/L obtained from the crustacean chronic toxicity 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.

Hazard Assessment（Basis for PNEC）			Assessment factor	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	10	0.9	Freshwater	0.017	0.02	○	○
					Seawater	<0.0021	<0.002		

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	Though a risk characterization cannot be determined, there would be little necessity of collecting information.	(○)
Ecological risk	No need of further work at present.		○

［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.