1	CAS No.: 98-82-8	Substance: Isopropylbenzene

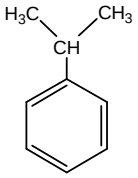
Chemical Substances Control Law Reference No.: 3-22 (Branched alkylbenzene (C3-36))

PRTR Law Cabinet Order No.:

Structural Formula:

Molecular Formula: C_9H_{12}

Molecular Weight: 120.19



1. General information

The aqueous solubility of this substance is 61.3 mg/L (25°C) and the partition coefficient (1-octanol/water) (log Kow) is 3.55 (23°C). The vapor pressure is 4.50 mmHg (= 600 Pa) (25°C). This substance is determinated to be ready biodegradable, but does not have hydrolizable groups.

The substance is mainly used in organic synthesis and production aviation gasoline, and for raw materials for peroxides and pro-oxidants. The total of production (shipment) and imports in FY 2001 was 100,000 to less than 1,000,000 tons/yr, and in FY 2004, 100,000 to less than 1,000,000 tons/yr as branched alkybenzene (C=3-36). The exports and imports in FY 2005 were 241,323 tons and zero tons, respectively.

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2. Exposure assessment

As isopropylbenzene is not 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. When predictions of distribution ratios by medium were made using the Mackay-Type Level III Fugacity Model, in the event of equal release to the atmosphere, water, and soil, the distribution ratio was highest for soil and water.

No predicted maximum exposure concentration for inhalation exposure to human beings could be established. The expected maximum concentration in the indoor air was 12 μg/m^3. The predicted maximum oral exposure was estimated to be less than 0.0004 μg/kg/day. The risk of exposure to this substance through food in environmental media is considered to be low.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was estimated to be approximately 0.03 μg/L for freshwater and approximately 0.01 μg/L for seawater public water bodies.

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3. Initial assessment of health risk

This substance is irritating to the eyes and the skin. Swallowing the liquid may cause aspiration into the lungs with the risk of chemical pneumonitis. Contact with eyes and skin may cause redness and pain, and dry skin, respectively. By inhalation or ingestion, it may cause dizziness, ataxia, drowsiness, headache and unconsciousness. There is a report that determined the toxic concentration lowest (TCLo) to be 200ppm（984 mg/m^3, drowsness, depressed activities and irritability）in human.

There was insufficient information regarding the carcinogenicity of the substance. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

A no observed adverse effect level (NOAEL) of 154 mg/kg/day (increase in the weight of kidneys of female) was obtained for oral exposure from the medium- and long-term toxicity testing for rats. The NOAEL was adjusted to 110 mg/kg/day taking into account the exposure situations. The value was divided by 10, because of the experimental period being short, and a value of 11 mg/kg/day was derived as the 'Non-toxic level*'. A no observed adverse effect level

(NOAEL) for the inhalation of 492 mg/m^3 (increase in the weight of liver, decrease in locomotor activity) was obtained from the medium- and long-term toxicity testing for rats. The NOAEL was adjusted to 88 mg/m^3 taking into account the exposure situation. The value was divided by 10, because of the experimental period being short, and a value of 8.8 mg/m^3 was derived as the 'Non-toxic level*'.

With regard to oral exposure, in case of groundwater intakes, the predicted maximum exposure was approximately less than 0.0004 μg/kg/day. The margin of exposure (MOE) of exceeding 2,800,000 was derived from the 'Non-toxic level*' of 11 mg/kg/day divided by the predicted maximum dose, and divided by 10, because the 'Non-toxic level*' was established by means of animal testing. As the exposure to this substance through food intakes was estimated minor, even when the exposure through groundwater and food are combined, it would not greatly affect the MOE values. Accordingly, further action for assessment of its health risk from oral exposure to this substance would not be required at present.

Concerning inhalation exposure to this substance in the ambient air, because the exposure concentrations have not been estimated, its health risk can not be identified. Concerning inhalation exposure to this substance in the indoor air, the predicted maximum exposure was 12μg/m^3. The MOE of 73 was derived from the 'Non-toxic level*' of 8.8 mg/m^3 divided by the predicted maximum exposure concentration, and divided by 10, because the 'Non-toxic level*' was established by means of animal testing. The substance is listed as a potential hazardous air pollutant, and has relatively high production volume. Its half-life in the atmosphere was estimated 9.8-98 hrs. This substance released into the atmosphere was estimated to distribute almost only into the atmosphere. Accordingly, it would be required to collect information on inhalation exposure to this substance in the ambient air and the indoor air for the assessment of its health risk.

Information of toxicity				Exposure assessment		Result of risk assessment			Judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	'Non-toxic level*' 11 mg/kg/day	Rats	increase in the weight of kidneys of female	Drinking water	— μg/kg/day	MOE	—	×	○
				Groundwater	< 0.0004 μg/kg/day	MOE	> 2,800,000	○	
Inhalation	'Non-toxic level*' 8.8 mg/m^3	Rats	increase in the weight of liver, decrease in locomotor activity	Ambient air	— μg/m^3	MOE	—	×	(▲)
				Indoor air	12 μg/m^3	MOE	73	▲	▲

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.

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4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 72-hour median effective concentration (EC_{50}) growth inhibition value of 2,600 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 24-hour median inhibition concentration (IC_{50}) immobilization value of 1,400 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour median lethal concentration (LC_{50}) value of 2,700 μg/L was found for the fish *Oncorhynchus mykiss* (rainbow trout). Accordingly, an assessment factor of 100 was used and a predicted no effect concentration (PNEC) of 14 μg/L was obtained based on the acute toxicity values. As no reliable information regarding chronic toxicity could be obtained, as the PNEC for the substance, a value of 14 μg/L obtained from the acute toxicity for the crustacea was used.

The PEC/PNEC ratio was 0.002 for freshwater bodies and 0.0007 for seawater bodies. 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	Result of assessment
Species	Acute / chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacea (water flea)	Acute	IC_{50} immobilization	100	14	Freshwater	0.03	0.002	○
					Seawater	0.01	0.0007	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	It would be required to collect information on inhalation exposure to this substance in the ambient and indoor air to assess its health risk.	▲
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

（○）: Though a risk characterization cannot be determined, there would be little necessity of collecting information.

（▲）: Further information collection would be required for risk characterization.