1	CAS No.: 98-82-8	Substance: Isopropyl benzene

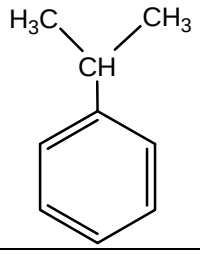
Chemical Substances Control Law Reference No.: 3-22 (branched alkyl benzene (C=3–36))

PRTR Law Cabinet Order No.: 1-83

Molecular Formula: C_9H_{12}

Molecular Weight: 120.19

Structural Formula:



1. General information

The aqueous solubility of this substance is 50 mg/1,000 g, the partition coefficient (1-octanol/water) (log K_{ow}) is 3.55 (23°C), and the vapor pressure is 4.6 mmHg (= 610 Pa) (25°C). Biodegradability (aerobic degradation) is judged to be good. The substance does not have any hydrolyzable groups.

This substance is designated as a Priority Assessment Chemical Substance and 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). The main uses of this substance are as a raw material for phenol and acetone, a gasoline additive, and a raw material for oxidants. The production and import quantity in fiscal 2012 was 847,311 t. The production and import category under the PRTR Law is more than 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2012 under the PRTR Law was approximately 176 t, of which approximately 159 t or 91% of overall releases were reported. The major destination of reported releases was the atmosphere. In addition, approximately 218 t was transferred to waste materials. The main source of reported releases was the chemical industry. The largest release among releases to the environment including those unreported was to the atmosphere. A multi-media model used to predict the proportions distributed to individual media in the environment indicated that in regions where the largest quantities were estimated to have been released to the environment overall or to the atmosphere in particular, the predicted proportion distributed to the atmosphere was 89.3%. In regions where the largest estimated releases were to public water bodies, the predicted proportion distributed to the atmosphere was 83%. In regions where the largest estimated releases were to soil, the predicted proportions distributed to soil and the atmosphere were 76.8% and 23%, respectively.

The maximum expected concentration of exposure to humans via inhalation, based on ambient air, was around 0.36 μg/m^3. In addition, the maximum expected concentration of exposure for indoor air was around 3.9 μg/m^3. However, albeit past data, the maximum for indoor air was 12 μg/m^3. The mean annual value for atmospheric concentration in fiscal 2012 was calculated by using a plume-puff model on the basis of releases to the atmosphere reported according to the PRTR Law; this model predicted a maximum level of 6.2 μg/m^3.

The maximum expected oral exposure could not be obtained. However, a value of around 0.0012 μg/kg/day was obtained from calculations based on past data for public freshwater. Although the measurement findings for public freshwater bodies are data from more than ten years ago, the likelihood of a more than single digit increase in public freshwater body concentrations is considered low when comparing the fiscal 2001 production (shipment) and import quantity (100,000 to <1,000,000 t) and the fiscal 2012 production and import quantity (847,311 t). The exposure level to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on the basis of its physicochemical properties.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained. However, albeit past data, values of around 0.03 μg/L for public freshwater bodies and around 0.01 μg/L for seawater have been obtained. Although the measurement findings for public freshwater bodies and seawater are data from more than ten years ago, the likelihood of a more than single digit increase in public freshwater body and seawater concentrations is considered low when comparing the fiscal 2001 production (shipment) and import quantity (100,000 to <1,000,000 t) and the fiscal 2012 production and import quantity (847,311 t).

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3. Initial assessment of health risk

This substance is irritating to the eyes and skin. Chemical pneumonitis may occur if the substance is swallowed in its liquid form and reaches the lungs. Contact of the substance with the eyes may cause redness and pain, while contact with the skin may cause dry skin. When inhaled or ingested, dizziness, ataxia, lethargy, headache and loss of consciousness may occur.

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

With regard to the oral exposure to the substance, the NOAEL of 154 mg/kg/day (based on kidney weight increase in female rats), resulting from mid-term and long-term toxicity tests on rats, was adjusted according to the test conditions to obtain an oral exposure of 110mg/kg/day, and divided by a factor of 10 due to the short test periods. The outcome of 11 mg/kg/day was considered to be the reliable lowest dose of the substance and was identified as its 'non-toxic level*'. As for the inhalation exposure to the substance, the NOAEL of 492 mg/m^3 (based on liver weight increase and locomotor activity decline) resulting from mid-term and long-term toxicity tests on rats, was adjusted according to the test conditions to obtain the exposure of 88mg/m^3; and was divided by a factor of 10 due to the short period. The outcome of 88 mg/m^3 was considered to be the reliable lowest dose of the substance and was identified as its 'non-toxic level*'.

Concerning the oral exposure to the substance, the absence of information available on exposure concentrations did not allow the health risk assessment. Nonetheless, the oral exposure level was estimated to be approximately 0.0012 μg/kg/day, according to the maximum concentration in public water bodies and freshwater, as reported in 2000. The MOE (Margin of Exposure) of 920,000 was derived from the oral exposure level and the 'non-toxic level*'of 11 mg/kg/day, after the division by a factor of 10 to convert animal data to human data. As exposure to the substance in the environment through diet is limited, the MOE would not change significantly even when this exposure is included. Therefore, collection of further information would not be required to assess the health risk of this substance for the oral exposure.

Regarding the inhalation exposure to the substance, the predicted maximum exposure concentration in ambient air was approximately 0.36 μg/m^3. The MOE of 2,400 was derived from the substance's 'non-toxic level*' of 8.8 mg/m^3 and the predicted maximum exposure concentration, and divided by 10 to convert animal data to human data. In addition, the MOE of 140 was derived from the maximum value of the atmospheric concentrations in the high discharging plants area of 6.2μg/m^3 (annual mean), calculated according to the reported emissions in the atmosphere in FY 2012 under the PRTR Law. Moreover, the predicted maximum exposure concentration in indoor air is approximately 3.9μg/m^3, and the MOE derived from this level would be 230. Therefore, no further action would be required at present to assess the health risk for the inhalation exposure in both ambient and indoor 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*' 11 mg/kg/day	Rat	Kidney weight increase in female rats	Drinking water	− μg/kg/day	MOE	−	×	(○)
				Groundwater	− μg/kg/day	MOE	−	×	

Inhalation	'Non-toxic level*' 8.8 mg/m^3	Rat	Liver weight increase and locomotor activity decline	Ambient air	0.36 μg/m^3	MOE	2,400	○	○
				Indoor air	3.9 μg/m^3	MOE	230	○	○

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 2,010 μg/L for growth inhibition in the green alga *Desmodesmus subspicatus*, a 24-h IC_{50} of 14,000 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 2,700 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 14 μg/L was obtained.

With regard to chronic toxicity, the following reliable datum was obtained: a 21-d NOEC of 350 μg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 3.5 μg/L was obtained.

The value of 3.5 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC of this substance could not be obtained. As such, a judgment on ecological risk could not be made. However, past data yielded values of around 0.03 μg/L for public freshwater bodies and around 0.01 μg/L for seawater, resulting in a ratio to PNEC of less than 0.01. Although public water body concentrations for this substance have not been obtained in recent years, the likelihood of a more than single digit increase in public freshwater body and seawater concentrations is considered low when comparing the current production and import quantity to those of fiscal 2001. Accordingly, the need to collect further data on this substance is considered to be minimal.

Hazard assessment (basis for PNEC)			Assessment coefficient	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/PNEC ratio	Judgment based on PEC/PNEC ratio	Assessment result
Species	Acute/ chronic	End point			Water body	Predicted environmental concentration PEC (μg/L)			
Crustacean *Daphnia magna*	Chronic	NOEC reproductive inhibition	100	3.5	Freshwater	–	–	×	○
					Seawater	–	–		

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Although risk to human health could not be confirmed, collection of further information would not be required.	(○)
	Inhalation exposure	No need for further work at present.	○
Ecological risk	No need for further work at present.		○

[Risk judgments] ○: No need for further work ▲: Requiring information collection

■: Candidates for further work ×: Impossibility of risk characterization

(○) : Although risk to human health could not be confirmed, collection of further information would not be required.

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