2	CAS No.: 4098-71-9	Substance: 3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate

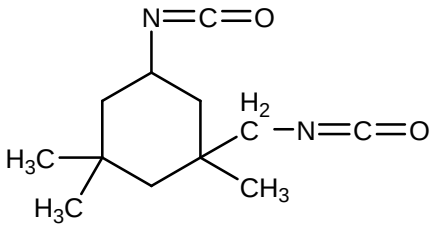
Chemical Substances Control Law Reference No.: 3-2492

PRTR Law Cabinet Order No.: 1-34

Molecular Formula: $C_{12}H_{18}N_2O_2$

Molecular Weight: 222.28

Structural Formula:



1. General information

The aqueous solubility of this substance is approximately 15 mg/L (23°C, this substance hydrolyzes rapidly), and its half-life for hydrolysis is approximately 1 h. The vapor pressure is 4.76×10^{-4} mmHg (0.0635 Pa) (20°C). This substance determinated to be persistent but not highly bioaccumulative.

This substance is designated 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). This substance is a major raw material for polyurethane. Polyurethane itself is used in urethane foam, coatings, elastomers (hand cart wheels, conveyor belts, etc.), and adhesives. The production and import quantity in fiscal 2013 was 3,000 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 2013 under the PRTR Law was approximately 0.043 t, and all releases were reported. All reported releases were to the atmosphere. In addition, 0.0002 t was transferred to sewage and approximately 16 t was transferred to waste materials. Industry types with large reported releases were the chemical industry and plastic product manufacturing industry. The largest release among releases to the environment including those unreported was to the atmosphere. A multi-media distribution prediction was not carried out because the required physicochemical properties could not be obtained.

The maximum expected concentration of exposure to humans via inhalation, based on general environmental atmospheric data, was around less than 0.002 μg/m^3. The mean annual value for the atmospheric concentration was calculated by using a plume-puff model on the basis of releases to the atmosphere in fiscal 2013 reported according to the PRTR Law; this model predicted a maximum level of 0.0063 μg/m^3. The maximum expected concentration of exposure to humans via oral intake could not be obtained. The likelihood of exposure to this substance by oral intake from an environmental medium is considered nonexistent for normal activities when taking into consideration the high hydrolyzability of this substance, PRTR data, etc.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be set because water quality data could not be obtained. The likelihood of exposure of aquatic organisms to this substance from water is considered nonexistent for normal activities when taking into consideration the high hydrolyzability of this substance, PRTR data, etc.

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3. Initial assessment of health risk

This substance is corrosive to the skin and causes redness, pain and serious skin burns. Its aerosol is irritating to the respiratory tract, and causes coughs, sore throat and burning sensation, if inhaled. Oral exposure to the substance causes sore throat, burning sensation and abdominal pain. Contact with the eyes is severely irritating,

and causes redness and pain.

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

The 'non-toxic level*' for oral exposure could not be identified.

The NOAEL of 0.27 mg/m^3 for inhalation exposure (based on epithelial changes in the nasal cavity and the larynx) determined from medium-term and long-term toxicity tests in rats, was adjusted for exposure conditions to obtain 0.048 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from sub-chronic to chronic exposure. The calculated value of 0.0048 mg/m^3 was deemed to be the lowest reliable concentration and was identified as the 'non-toxic level*' of the substance for inhalation exposure.

With regard to oral exposure, owing to lack of identified 'non-toxic level*' and exposure levels, the health risk could not be assessed. Nonetheless, considering that the total amount of the substance released to the environment was 0.043 t; that all of it was emitted to ambient air, and the half-life of the substance in water is estimated to be approximately 1 hour, collection of further information would not be required to assess the health risk of this substance via oral exposure.

With regard to inhalation exposure, the predicted maximum exposure concentration in ambient air was less than 0.002 μg/m^3, approximately. The MOE (Margin of Exposure) would be over 240, when calculated from the predicted maximum exposure concentration and the 'non-toxic level*'of 0.0048 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans.

In addition, the maximum concentration (annual mean) in ambient air near the operators releasing large amount of the substance to ambient air was estimated to be 0.0063 μg/m^3 on the basis of the data reported in FY 2013 under the PRTR Law. The MOE would be 76, when calculated from this value and the 'non-toxic level*'.

Therefore, collection of further information on exposure would be required to assess the health risk of this substance via inhalation in 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*' — mg/kg/day	—	—	Drinking water	— μg/kg/day	MOE	—	×	(○)
				Groundwater	— μg/kg/day	MOE	—	×	
Inhalation	'Non-toxic level*' 0.0048 mg/m^3	Rat	Epithelial changes in the nasal cavity and the larynx	Ambient air	<0.002 μg/m^3	MOE	>240	○	(▲)
				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

This substance is used as a curing agent for polyurethane resin. Total release to the environment reported under the PRTR law was 0.043 t, all of which was to the atmosphere. However, the likelihood of detecting this substance released to the atmosphere in public water bodies is considered nonexistent when taking into account its high hydrolyzability (half-life of approximately 1 h) and measured values in the general environmental atmosphere. Although releases to the environment from the transfer of this substance contained in waste materials transported from sites handling it (approximately 16 t) are unclear, its high hydrolyzability (half-life is approximately 1 h) means that for normal activities, the likelihood of exposure to this substance from water for aqueous organisms is considered nonexistent.

In addition, the toxicity value for this substance obtained from toxicity test findings for aqueous organisms is thought to indicate the toxicity of its hydrolysis products, and not reflect the actual toxicity of the substance.

Accordingly, an initial assessment of ecological risk to aqueous organisms for this substance was not conducted.

A separate evaluation of the need for an initial assessment of the ecological risk of this substance's hydrolysis products is considered necessary.

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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	Further information collection would be required for risk characterization.	(▲)
Ecological risk	Initial assessment of ecological risk to aqueous organisms for this substance was not carried out. Another evaluation of the need for an initial assessment of ecological risk of substance's hydrolysis products considered necessary.		(－)

［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.