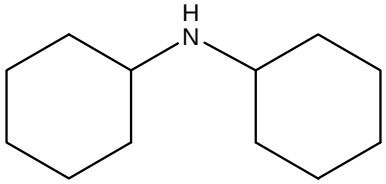
6	CAS No.: 101-83-7	Substance: *N*,*N*-Dicyclohexylamine

Chemical Substances Control Law Reference No.: 3-2259 (Dicyclohexylamine), 3-2686 (Dicyclohexylamine)
PRTR Law Cabinet Order No.: 1-188
Molecular Formula: $C_{12}H_{23}N$
Molecular Weight: 181.32

Structural Formula:



1. General information

The aqueous solubility of this substance is 800 mg/L (calculated value), the partition coefficient (1-octanol/water) (log K_{ow}) is 2.724 (25°C), and the vapor pressure is 0.02 mmHg (3 Pa) (25°C). Biodegradability (aerobic degradation) is judged to be good. The substance does not have any hydrolyzable groups under environmental conditions.

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). The main use of this substance is as a raw material for rust inhibitors, rubber chemicals, surfactants, and dyestuffs. The production and import quantity in fiscal 2013 was 2,000 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 10 t, of which approximately 7.4 t or 73% of overall releases were reported. The major destination of reported releases was the atmosphere. In addition, approximately 6.4 t was transferred to sewage and approximately 170 t was transferred to waste materials. Industry types with large reported releases were metal product manufacturing and transportation equipment manufacturing for the atmosphere, and steel making and transportation equipment manufacturing for public water bodies. The largest release among releases to the environment including those unreported was to water bodies.

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 the atmosphere in particular, the predicted proportion distributed to the atmosphere was 39.4%, that distributed to water bodies was 34.4%, and that distributed to soil was 23.5%. In regions where the largest quantities were estimated to have been released to public water bodies, the predicted proportion distributed to water bodies was 98.5%. In regions where the largest quantities were estimated to have been released to soil, the predicted proportion distributed to water bodies was 63.3% and that distributed to soil was 28.3%.

The maximum expected concentration of exposure to humans via inhalation, based on general environmental atmospheric data, was less than around 0.009 μg/m^3. The mean annual value for the atmospheric concentration in fiscal 2013 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 0.79 μg/m^3. The predicted maximum oral exposure was estimated to be less than around 0.2 μg/kg/day when calculated from data for food. Furthermore, the predicted maximum exposure calculated from food and past data for public freshwater bodies was more than around 0.008 μg/kg/day and less than around 0.2 μg/kg/day. In contrast, when releases to public freshwater bodies in fiscal 2013 reported according to the PRTR Law were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only

dilution gave a maximum value of 3.6 μg/L. Using this estimated concentration for rivers to calculate oral exposure gave 0.14 μg/kg/day.

Information to determine the predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained. However, values of around 0.2 μg/L for public freshwater and generally 0.03 μg/L for seawater were obtained from calculations based on past data. When releases to public freshwater bodies in fiscal 2013 reported according to the PRTR Law were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 3.6 μg/L.

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3. Initial assessment of health risk

This substance is corrosive to the eyes, skin and respiratory tract. Inhalation of the substance causes sore throat, coughs, burning sensation, shortness of breath and labored breathing, and inhalation of its vapor may cause lung edema. Oral exposure to the substance causes burning sensation, abdominal pain and shock or collapse. Contact with the eyes or skin causes pain, redness and burns.

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 NOAEL of 20 mg/kg/day for oral exposure (based on salivation and convulsion), determined from the medium-term and long-term toxicity tests in rats, was divided by a factor of 10 to account for extrapolation from sub-acute to chronic exposure. The obtained value of 2.0 mg/kg/day was deemed to be the lowest reliable dose and was identified as the 'non-toxic level*' of the substance for oral exposure.

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

With regard to oral exposure, assuming the substance is ingested via public freshwater bodies and food, the predicted maximum exposure level was less than 0.2 μg/kg/day approximately. The MOE (margin of exposure) would be over 1,000, when calculated from the predicted maximum exposure level and the 'non-toxic level*'of 2.0 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. The maximum exposure level of the substance ranged from 0.008 μg/kg/day to 0.2 μg/kg/day approximately on the basis of the data on food and public freshwater bodies in 2001, and the MOE derived from this exposure range and the 'non-toxic level*' was within the range of 1,000 to 25,000.

In addition, the maximum exposure level was calculated to be 0.14 μg/kg/day. This value derives from the concentration in effluents from high discharging plants, estimated according to the emissions data reported in FY 2013 under the PRTR Law. The MOE derived from this value and the 'non-toxic level*' was 1,400.

Therefore, no further work would be required at present to assess the health risk of this substance via oral exposure.

With regard to inhalation exposure, owing to lack of identified 'non-toxic level*', the health risk could not be assessed. For comparison, assuming that 100% of the ingested substance is absorbed, the 'non-toxic level*' of inhalation exposure, derived by converting that of oral exposure, would be 6.7 mg/m^3. The MOE would be over 74,000, when calculated from this value and the predicted maximum exposure concentration of less than 0.009 μg/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 0.79 μg/m^3 on the basis of the data reported in FY 2013 under the PRTR Law. The MOE would be 850, when calculated from the maximum concentration in ambient air and the 'non-toxic level*'.

Therefore, collection of further information would not 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*' 2.0 mg/kg/day	Rat	Salivation and convulsion	Drinking water	— μg/kg/day	MOE	—	×	○
				Food	<0.2 μg/kg/day	MOE	>1,000	○	
Inhalation	'Non-toxic level*' — mg/m^3	—	—	Ambient air	<0.009 $\mu g/m^3$	MOE	—	×	(○)
				Indoor air	— $\mu g/m^3$	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

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC_{50} exceeding 19,400 μg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, a 48-h of EC_{50} of 8,000 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 12,000 μg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 80 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 2,030 μg/L for growth inhibition in the green algae *P. subcapitata* and a 21-d NOEC of 49 μg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 0.49 μg/L was obtained.

The value of 0.49 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

Information to determine 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 0.2 μg/L for freshwater bodies and generally 0.03 μg/L for seawater. Hence, the PEC/PNEC ratio is 0.4 for freshwater bodies and 0.06 for seawater. This substance was officially published in the sixth revision (2008) but no new data were obtained to necessitate a change in the PNEC value. In the meantime, based on enactment of the PRTR Law in 2009, when releases to public freshwater bodies in fiscal 2013 reported according to the PRTR Law were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 3.6 μg/L, yielding a PEC/PNEC ratio of 7.3. Regarding this substance, efforts are needed to precisely evaluate its production and import quantity as well as its applications, and to enhance the information regarding its environmental concentrations and ecological effects as needed.

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	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)			
Crustacean *Daphnia magna*	Chronic	NOEC reproductive inhibition	100	0.49	Freshwater	−	−	×	▲
					Seawater	−	−		

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5. Conclusions

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

［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.