13	CAS No: 108-45-2	Substance: *m*-Phenylenediamine

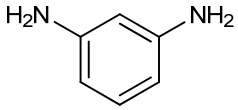
Chemical Substances Control Law Reference No.: 3-185 (phenylenediamine)

PRTR Law Cabinet Order: 1-348 (phenylenediamine)

Molecular Formula: $C_6H_8N_2$

Molecular Weight: 108.14

Structural Formula:



1. General information

The aqueous solubility of this substance is 3.48×10^4 mg/1,000g (20°C), the partition coefficient (1-octanol/water) (log K_{ow}) is -0.33 (pH = 7.4), and the vapor pressure is 4×10^{-3} mmHg (= 0.5 Pa) (20°C). Biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 2% and bioaccumulation is judged to be non-existent or low.

This substance is designated as a Priority Assessment Chemical Substance. Phenylenediamine is also 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 dyestuffs (azo dyestuffs, hair dyes, mordants), rubber additives, and high performance fibers or heat-resistant polymers, and as a curing agent for epoxy resin among other uses. The production and import quantity in fiscal 2012 was 998 t. The production and import category under the PRTR Law for phenylenediamine is more than 100 t.

---

2. Exposure assessment

Total release of phenylenediamine to the environment in fiscal 2012 under the PRTR Law was approximately 5.1 t, of which approximately 3.3 t or 64% of overall releases were reported. The major destination of reported releases was public water bodies. In addition, approximately 37 t was transferred to waste materials, and approximately 2.1 t was transferred to sewage. Industry types with large reported releases were plastic product manufacturing for the atmosphere and the chemical industry alone 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 to public water bodies in particular, the predicted proportion distributed to water bodies was 98.3%. In regions where the largest estimated releases were to the atmosphere, the predicted proportion distributed to water bodies was also 98.3%.

The maximum expected concentration of exposure to humans via inhalation could not be obtained. The mean annual value for atmospheric concentration in fiscal 2012 was calculated by using a plume-puff model on the basis of releases (as phenylenediamine) to the atmosphere reported according to the PRTR Law; this model predicted a maximum level of 0.021 μg/m^3. The maximum expected oral exposure was estimated to be around less than 0.0004 μg/kg/day on the basis of calculations from data for public freshwater bodies. When releases (as phenylenediamine) to public freshwater bodies in fiscal 2012 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 0.041 μg/L. Using this estimated concentration for rivers to calculate oral exposure gave 0.0016 μg/kg/day. The exposure level to this substance by intake from an environmental medium via food is considered slight, based on its low bioaccumulation.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around less than 0.01 μg/L for both public freshwater bodies and seawater. When releases (as phenylenediamine) to public freshwater bodies in fiscal 2012 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 0.041 μg/L.

---

3. Initial assessment of health risk

This substance irritates the eyes and skin. The substance may possibly affect the kidneys and blood, causing kidney failure and producing methemoglobin. When inhaled or ingested, cyanosis of lips, nail beds and skin, confusion, convulsion, dizziness, nausea and loss of consciousness may occur. Contact of the substance with the skin may cause redness, while contact with the eyes may cause redness and pain.

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 2.2 mg/kg/day (based on body weight gain inhibition), obtained for mid-term and long-term toxicity tests on rats, 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 'non-toxic level* could not be identified.

With regard to the oral exposure to the substance, the predicted maximum exposure level was below 0.0004 μg/kg/day, assuming ingestion of water from public water bodies and freshwater. The MOE (Margin of Exposure) of more than 550,000 was derived from the substance's 'non-toxic level*' of 2.2 mg/kg/day and the predicted maximum exposure level, after the division by a factor of 10 to convert animal data to human data. In addition, the MOE of 140,000 was derived from the substance's maximum exposure concentration of 0.0016 μg/kg/day according to the concentrations of the substance (as Phenylenediamine) in effluents from high discharging plants reported in FY 2012 under the PRTR Law. 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, no further work would be required at present to assess the health risk for the oral exposure to this substance.

Concerning the inhalation exposure to the substance, the health risk could not be assessed as its 'non-toxic level*' could not be established, nor the exposure concentrations. In addition, assuming a 100 % absorption, and converting the 'non-toxic level*' for oral exposure to the inhalation one, the 'non-toxic level*' would be 7.3 mg/m^3. The MOE of 35,000 was derived from this level and the maximum atmospheric concentration in the high discharging plants area of 0.021 $\mu g/m^3$ (annual mean), calculated from the emissions reported (as Phenylenediamine) in FY 2012 under the PRTR Law and after the division by a factor of 10 to convert animal data to human data. Therefore, collection of information would not be required to assess the health risk for the inhalation exposure to this substance 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*' 2.2 mg/kg/day	Rat	Body weight gain inhibition	Drinking water	– μg/kg/day	MOE	–	×	○
				Freshwater	<0.0004 μg/kg/day	MOE	>550,000	○	
Inhalation	'Non-toxic level*' – mg/m^3	–	–	Ambient air	– $\mu g/m^3$	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.

4.Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 96-h EC_{50} of 2,400 µg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*, a 48-h EC_{50} of 2,000 µg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} exceeding 100,000 µg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a PNEC of 20 µg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 96-h NOEC of 915 µg/L for growth inhibition in the green alga *P. subcapitata*, and a 21-d NOEC of 50 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 0.5 µg/L was obtained.

The value of 0.5 µg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio is less than 0.02 for both freshwater bodies and seawater. In addition, the river concentration (as phenylenediamine) estimated by using releases reported according to the PRTR Law and taking only dilution into consideration gives 0.041 µg/L, resulting in a ratio to PNEC of less than 0.1. Accordingly, further work on this substance is considered unnecessary at this time.

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	0.5	Freshwater	<0.01	<0.02	○	○
					Seawater	<0.01	<0.02		

---

5. Conclusions

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