

11	CAS No.: 91-76-9	Substance: 6-Phenyl-1,3,5-triazine;2,4-diamine
Chemical Substances Control Law Reference No.:5-1028 PRTR Law Cabinet Order No.: Molecular Formula: C ₉ H ₉ N ₅ Structural formula: Molecular Weight: 187.20		

1. General information

The water solubility of this substance is 320 mg/L (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 1.38 (25°C), and the vapor pressure is less than 3.1×10⁻⁷ mmHg (less than 4.1×10⁻⁵ Pa) (100°C). In the aerobic biodegradation test, BOD degradation rate was 2%. This substance is judged not to be bioaccumulative. The hydrolysis half-life exceeds 5 days (pH=4, 7, 9, 50°C).

The main use is as a benzoguanamine-formaldehyde resin intermediate. The production and import quantity in FY 2009 was 2,555 t.

2. Exposure assessment

Because this substance is not classified as a Class 1 Designated Chemical Substance 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. Predictions of distribution by medium using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to soil would be greater.

The predicted maximum exposure to humans via inhalation, based on general environmental atmospheric data, was around 0.00017 µg/m³. The predicted maximum oral exposure was estimated to be around 0.00048 µg/kg/day based on calculations from data for public fresh water bodies. Further, an environmental study of a limited area reported a value of 0.00064 µg/kg/day calculated from data for public freshwater bodies. The risk of exposure to this substance by intake from an environmental medium via food is considered slight based on estimates of oral exposure using estimated concentrations in fish.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.012 µg/L for public freshwater bodies and around 0.0098 µg/L for seawater. Further, there is a report of around 0.016 µg/L for public freshwater bodies, albeit based on an environmental survey of a limited area.

3. Initial assessment of health risk

This substance is slightly irritating to eyes, and contact with it makes eyes red. When the substance was orally administered to rats, mucosal hypertrophy and edema in submucosal tissue were observed for forestomach of dead animals. In addition, white spots over mucosa of forestomach and hyperplasia of squamous epithelium were noted for surviving animals.

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

As for oral exposure to the substance, a NOAEL of 4 mg/kg/day (for suppressed body weight increase and tremor) obtained from mid- and long-term toxicity tests on rats was divided by 10 due to their rather short test periods. Its outcome of 0.4 mg/kg/day was deemed to be the lowest reliable dose without any effect, and this was identified as its 'non-toxic level*'. As for inhalation exposure to the substance, its 'non-toxic levels*' could not be identified.

As for its oral exposure, its mean exposure would be about 0.00014 µg/kg/day and its predicted maximum exposure

would be around 0.00048 µg/kg/day, respectively, if its intakes through freshwater from public water bodies and through soil were assumed. The MOE would be 83,000 when calculated from the ‘non-toxic level*’ of 0.4 mg/kg/day and the predicted maximum exposure, and divided by 10 for conversion of the ‘non-toxic level*’ from animal experiments to an equivalent dose for humans. For reference, its maximum exposure of 0.00064 µg/kg/day has been reported for freshwater from public water bodies for some location, and this will provide MOE of 63,000. Since risk of exposure to this substance through food intakes from the environment would be limited, even when this exposure were combined, significant changes in the MOE would not be likely. Therefore, further actions would not be required at the moment to assess health risk from oral exposure to this substance.

As for its inhalation exposure, lack of available information on its ‘non-toxic levels*’ did not allow its health risk assessment. For reference, if 100% absorption were assumed, its ‘non-toxic level*’ for oral exposure would be converted to its ‘non-toxic level*’ of 1.3 mg/m³ for inhalation exposure. The MOE would be 760,000 when calculated from its ‘non-toxic level’ of 1.3 mg/m³ and its predicted maximum concentration of 0.00017 µg/m³. Therefore, collection of information would not be required to assess health risk from inhalation exposure to the substance in the 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 * *	0.4 mg/kg/day	Rats	Suppressed body weight increase	Drinking water	—	µg/kg/day	MOE	—	×	○
					Freshwater	0.00048	µg/kg/day	MOE	83,000	○	
Inhalation	Non-toxic level * *	— mg/m ³	—	—	Ambient air	0.00017	µg/m ³	MOE	—	×	(○)
					Indoor air	—	µg/m ³	MOE	—	×	×

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.

4.Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC₅₀ of 70,600 µg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*; a 48-h EC₅₀ of 52,000 µg/L for immobilization in the crustacean *Daphnia magna*; and a 48-h LC₅₀ of 99,000 µg/L for the fish *Leuciscus idus* (Cyprinidae). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 520 µg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 39,100 µg/L for growth inhibition in the green algae *P. subcapitata*; and a 21-d NOEC of 1,910 µg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 19 µg/L was obtained. This 19 µg/L obtained from the crustacean chronic toxicity was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.0006 for freshwater bodies and 0.0005 for seawater. 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	Judgment based on PEC/PNEC ratio	Assessment result
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (µg/L)			
Crustacean <i>Daphnia magna</i>	Chronic	NOEC reproductive inhibition	100	19	Freshwater	0.012	0.0006	○	○
					Seawater	0.0098	0.0005		

5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	Though a risk characterization cannot be determined, there would be little necessity of collecting information.	(○)
Ecological risk	No need of further work at present.		○

[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.