8	CAS No.: 21564-17-0	Substance: 2-(Thiocyanatomethylthio)-1,3-benzothiazole

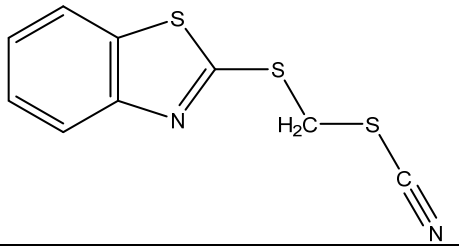
Chemical Substances Control Law Reference No.: 5-3424

PRTR Law Cabinet Order No.: 2-57

Molecular Formula: $C_9H_6N_2S_3$

Molecular Weight: 238.35

Structural Formula:



1.General information

The aqueous solubility of this substance is 125 mg/L (24°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 3.12, and the vapor pressure is 3.12×10^{-7} mmHg (=4.16×10^{-5} Pa) (25°C, calculated value). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and bioaccumulation is thought to be nonexistent or low.

This substance is classified as a Class 2 Designated Chemical Substance under the PRTR Law. The main use of this substance is as an antifungal agent for wood and leather. It is also used as a disinfectant for agricultural materials (seedling boxes, seedling pots, supports, etc.).

The production and import quantity in fiscal 2015 was not disclosed because the number of reporting businesses was not more than two. The production and import quantity in fiscal 2016 was more than 1 t and less than 100 t.

---

2. Exposure assessment

Because this substance is not classified as a Class 1 Designated Chemical Substance under the PRTR Law, release and transfer quantities could not be obtained. Predictions of proportions distributed to individual media by use of a Mackay-type level III fugacity model indicate that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to soil would be largest.

The maximum expected concentration of exposure to humans via inhalation could not be determined because ambient atmospheric and indoor air quality data could not be obtained.

Data for potable water, ground water, food and soil to assess oral exposure could not be obtained. Thereupon, assuming intake solely from public freshwater bodies, a maximum expected concentration of exposure of around less than 0.000033 μg/kg/day was obtained. Furthermore, a reference value of less than 0.021 μg/kg/day was obtained for maximum expected concentration of exposure based on data measured for public freshwater bodies and food, albeit for the latter surveyed over a limited area.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was reported to be around less than 0.00082 μg/L for public freshwater bodies and about 0.0011 μg/L for seawater.

---

3. Initial assessment of health risk

Inhalation of this substance causes cough. The substance is irritating to the skin and causes dryness, redness, roughness and burning sensation. The substance is corrosive to the eyes and causes redness, pain and severe deep 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 LOAEL of 3.8 mg/kg/day for oral exposure (based on decrease in leukocytes and monocytes), determined from toxicity tests in dogs, was divided by a factor of 10 to account for uncertainty in using a LOAEL. The calculated value of

0.38 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 absorbed via public freshwater bodies, the predicted maximum exposure level would be less than 0.000033 μg/kg/day, approximately. The MOE (Margin of Exposure) would exceed 1,200,000, when calculated from the predicted maximum exposure level and the 'non-toxic level*'of 0.38 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Assuming the substance is absorbed via food, which data is based on restricted area; and public freshwater bodies, the exposure level would be less than 0.021 μg/kg/day, approximately. The MOE would exceed 1,800, when calculated from this exposure level. 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 the lack of identified 'non-toxic level*' and exposure concentrations, the health risk could not be assessed. The vapor pressure of the substance is low, and predictions of the multimedia fugacity model indicated that the proportion distributed to air was little. The substance was not detected in samples collected from public freshwater bodies. Given these facts, the concentration of the substance in ambient air is not likely to become a major concern. 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*' 0.38 mg/kg/day	Dogs	Decrease in leukocytes and monocytes	Drinking water	- μg/kg/day	MOE	-	○
				Public freshwater bodies	<0.000033 μg/kg/day	MOE	>1,200,000	
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 48-h LC_{50} of 15.3 μg/L for the crustacean *Ceriodaphnia dubia* (water flea) and a 96-h LC_{50} of 11.5 μg/L for the fish species *Oncorhynchus tshawytscha* (Chinook salmon). Accordingly, based on these acute toxicity values and an assessment factor of 1,000, a predicted no effect concentration (PNEC) of 0.0115 μg/L was obtained.

With regard to chronic toxicity, the following reliable data was obtained: a 7-d NOEC of 2.5 μg/L for reproductive inhibition in the crustacean *C. dubia*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 0.025 μg/L was obtained.

The value of 0.0115 μg/L obtained from the acute toxicity to the fish species was used as the PNEC for this substance.

The PEC/PNEC ratio is less than 0.07 for freshwater bodies and 0.096 for seawater; accordingly, further work 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	Assessment result
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Fish *Oncorhynchus tshawytscha*	Acute	LC_{50} mortality	1,000	0.0115	Freshwater	<0.00082	<0.07	○
					Seawater	0.0011	0.096	

---

5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	No need for further work.	○
Ecological risk	No need for further work.		○

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

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

（▲）: Further efforts to collect data required based on comprehensive review of existing relevant data

（■）: Candidate for further work based on comprehensive review of existing data