11	CAS No ·	98-07-7

### Substance: Benzotrichloride

Chemical Substances Control Law Reference No.: 3-87

PRTR Law Cabinet Order No.: 1-397

Molecular Formula:C<sub>7</sub>H<sub>5</sub>Cl<sub>3</sub>

Molecular Weight: 195.47



## 1. General information

The vapor pressure of this substance is 2.6 mmHg (=350 Pa) ( $25^{\circ}$ C) and biodegradability (aerobic degradation) is judged to be good. Its half-life for hydrolysis is 11 s ( $25^{\circ}$ C, pH7).

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 UV absorbers, pharmaceuticals, agricultural chemicals, dyes, pigments and other organic compounds. The production (shipments) and import quantity in fiscal 2011 was 4,000 t. The production and import category under the PRTR Law is more than 100 t.

### 2. Exposure assessment

Total release to the environment in fiscal 2011 under the PRTR Law was 0.0001 t and all releases were reported. All reported releases were to the atmosphere. In addition, 3.9 t was transferred to waste materials. The only source of reported releases was the chemical industry. 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 generally less than  $0.004 \,\mu g/m^3$ . The mean annual value for the atmospheric concentration in fiscal 2011 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  $0.000016 \,\mu g/m^3$ . The maximum expected oral exposure could not be obtained. The possibility of oral exposure to this substance via an environmental medium is thought to be low when taking into consideration its high hydrolyzability and PRTR data.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained. The possibility of exposure to this substance via water is thought to be low when taking into consideration its high hydrolyzability and PRTR data.

# 3. Initial assessment of health risk

This substance may cause irritation to skin and respiratory tract, and it may cause severe irritation to eyes. Vomiting may occur when the substance is swallowed, and it may possibly cause aspiration pneumonia. Poisoning by its inhalation would lead to symptoms such as coughing, sore throat and shortness of breath.

With regard to non-carcinogenic health risk of the substance, information on its general toxicity on animals and its reproductive and developmental toxicity on them was available. As for its carcinogenicity, there were evidences of its carcinogenic effects on animals observed in their experiments. Therefore, an initial assessment was conducted on both non-carcinogenicity and carcinogenicity of the substance since it could be carcinogenic also to humans.

With regard to oral exposure to the substance, a LOAEL of 0.048 mg/kg/day (for degeneration of liver, kidney or thyroid tissue) obtained from its mid-term and long-term toxicity tests on rats was divided by a factor of 10 for conservative use of the LOAEL, and further divided by a factor of 10 for their short test periods. Outcome of

0.00048 mg/kg/day is deemed to be the reliable lowest dose. As no information on the threshold for its carcinogenicity was available, this 0.00048 mg/kg/day was deemed to be its 'non-toxic level\*' on the basis of its non-carcinogenic effects. When no threshold were assumed for its carcinogenicity,  $1.3 \times 10 \text{ (mg/kg/day)}^{-1}$  (for pulmonary adenocarcinoma) from experiments on mice would be its slope factor.

As for non-carcinogenic effects of its inhalation exposure, a NOAEL of 5.1 mg/m<sup>3</sup> (for symptoms such as suppressed body weight increase, nasal, bronchial/pulmonary inflammation or degeneration) obtained from its mid-term and long-term toxicity tests on rats was adjusted for their durations to provide 0.91 mg/m<sup>3</sup> for its intermittent to continuous exposure, and this was divided by a factor of 10 due to their short test periods. Outcome of 0.091 mg/m<sup>3</sup> was identified to be the reliable lowest dose of the substance and its 'non-toxic level\*'. As for its carcinogenicity, no information to identify its unit risk would be available if no threshold were assumed for its carcinogenicity.

With regard to oral exposure to the substance, its health risk could not be assessed as its exposure levels were not known. In addition, total releases of this substance to the environment in FY 2011 were 0.0001 t and all of them were emitted to the ambient air. Therefore, collection of further information would not be required to assess health risk of its oral exposure.

As for inhalation exposure to the substance, both its mean and maximum exposure concentrations were estimated to be below about 0.004  $\mu$ g/m<sup>3</sup>. The MOE (Margin of Exposure) would be over 230 when calculated from its predicted maximum exposure concentration and its 'non-toxic level\*' of 0.091 mg/m<sup>3</sup> and divided by a factor of 10 to convert animal data to human data, and further divided by a factor of 10 to extrapolate animal data to the carcinogenic hazard to humans. In addition, the MOE would be 57,000 when calculated for reference from its maximum (annual mean) exposure of 0.000016  $\mu$ g/m<sup>3</sup> in the ambient air near the operators discharging the substance in high concentrations reported in FY 2011 under the PRTR Law. Therefore, no further action would be required at this moment to assess health risk of its inhalation exposure in the ambient air.

Toxicity						Exposure assessment				
Exposu re Path	Criteria for risk as	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure dose and concentration		nent	Judgm ent		
Oral	'Non-toxic 0.00048	mg/kg/day	Rat	Lesions in liver, kidneys or thyroid	Drinking water	- μg/kg/day	MOE Excess incidenc e rate	-	×	( )
	Slope factor $1.3 \times 10$	(mg/kg/day) <sup>-1</sup>	Mouse	tissues	Ground water	- μg/kg/day	MOE - Excess incidenc - e rate	×		
	'Non-toxic 0.091	mg/m <sup>3</sup>	Rat	Suppressed body weight increase, nasal, bronchial/ pulmonary	Ambient air	<0.004 µg/m <sup>3</sup>	MOE Excess incidenc e rate	>230	×	
Inhalati on	Unit risk	(µg/m <sup>3</sup> ) <sup>1</sup>	-	inflammation or degeneration, etc. -	Indoor air	- μg/m³	MOE Excess incidenc e rate	-	×	×

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

This substance is used as a raw material for UV absorbers and other organic compounds. The total release to the environment in fiscal 2011 reported under the PRTR Law was 0.1 kg; all releases were to the atmosphere.

The possibility of detecting releases of this substance to the atmosphere in public water bodies is considered to be low, given its high hydrolyzability (half-life of 11 s) and concentration in typical atmospheric environments.

Release of this substance to the environment from the quantity transferred to waste materials (i.e., 3.9 t shipped from factories that handle the substance) is unclear. However, even if it were released to water systems, the likelihood of exposure to this substance via water would be low given its high hydrolyzability.

In addition, the toxicity values obtained from tests of this substance using aquatic organisms likely indicate the toxicity of its hydrolysis products and are unlikely to reflect the toxicity of the substance itself.

Therefore, although an initial assessment of the ecological risk could not be made, the likelihood of this substance itself affecting aquatic organisms is considered low. Accordingly, further work is considered unnecessary at this time.

ſ	Hazard asses	sment (basi	s for PNEC)	,	Predicted no effect concentration PNEC (µg/L)	Exposure assessment		DECIDNEC	Judgment	
	Species	Acute/ chronic	Endpoint	factor		Water body	Predicted environmental concentration PEC (µg/L)	ratio	PEC/PNEC ratio	result
						Freshwater	-	-		
-	-	-	-	-	Seawater	-	-	×		

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# 5. Conclusions

	Conclusions					
Health risk	Oral exposure	Although risk to human health could not be confirmed, collection of further information would not be required.	( )			
	Inhalation exposure	No need of further work at present.				
Ecological risk	No need of further work at present.					
[ Risk judgmer	nts] : No ne	eed for further work <b>A</b> : Requiring information collection				
	: Candi	dates for further work ×: Impossibility of risk characterization				
( ): Though a risk characterization cannot be determined, there would be little necessit						
	of collect	ing information.				
( $\blacktriangle$ ) : Further information collection would be required for risk characterization.						