11	CAS No: 96-18-4	Substance: 1,2,3-trichloropropane

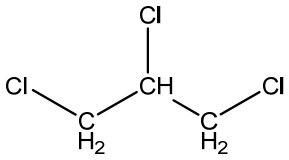
Chemical Substances Control Law Reference No.: 2-83（poly(3–5)chloropropane)

PRTR Law Cabinet Order: 1-289

Molecular Formula: $C_3H_5Cl_3$

Molecular Weight: 147.43

Structural formula:



1. General information

The aqueous solubility of this substance is 2×10^3 mg/1,000g (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 2.63, and the vapor pressure is 3.69 mmHg (= 492 Pa) (25°C). Biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and bioaccumulation is judged to be non-existent or low. Its half-life for hydrolysis is 44 years (calculated value).

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 uses of this substance are as a synthetic intermediate for pesticides and other chemical substances in closed systems and a cross-linking agent for chemicals such as polysulfides and hexafluoropropylene during the production of polymers. The production and import quantity of poly(3–5)chloropropane in fiscal 2012 was not disclosed because the number of reporting businesses was not more than two but it was 2000 t in fiscal 2011. The production and import category under the PRTR Law is 1 to < 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2012 under the PRTR Law was approximately 0.25 t, and all releases were reported. The sole destination of reported releases was the atmosphere. In addition, approximately 370 t was transferred to waste materials. The main source of reported releases was the chemical industry. 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 the atmosphere in particular, the predicted proportion distributed to the atmosphere was 88.3%.

The maximum expected concentration of exposure to humans via inhalation, based on ambient air, was around 0.059 μg/m^3. The mean annual value for atmospheric concentration 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 0.018 μg/m^3. The maximum expected oral exposure could not be obtained. However, albeit past data, a maximum expected exposure of around 0.0012 μg/kg/day was calculated from public freshwater body data. 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, could not be obtained. However, past data yielded values of 0.03 μg/L for freshwater bodies and around 0.01 μg/L for seawater.

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3. Initial assessment of health risk

This substance is irritating to the eyes and respiratory tract and may possibly affect the liver and kidney,

resulting in functional hepatic and renal disorder, and may cause loss of consciousness when exposure to high doses. When inhaled, coughing, sore throat, headache, lethargy and loss of consciousness may occur, while nausea, headache, vomiting, diarrhea, lethargy and loss of consciousness may occur when ingested. Contact of the substance with the eyes may cause redness and pain, while contact with the skin may cause dry skin, redness and stabbing pain.

With regard to the substance's non-carcinogenic health risk, information on general, reproductive and developmental toxicity was available. As for carcinogenicity of the substance, there was evidence on the carcinogenic effects for animal tests, and as carcinogenic effect is also suspected for humans, the initial assessment was conducted on both non-carcinogenic and carcinogenic risks.

With regard to the oral exposure for non-carcinogenic effects, the LOAEL of 3 mg/kg/day (based on liver weight increase, forestomach hyperplasia, etc.), resulting from mid-term and long-term toxicity tests on rats, was adjusted according to the test conditions, to obtain the exposure of 21 mg/kg/day and was divided by a factor of 10 for the use as a LOAEL. The outcome of 0.21 mg/kg/day was identified as the 'non-toxic level*' of the substance. As for the carcinogenic effects, the results of experiments on rats gave the level of 7 (mg/kg/day), determined as the slope factor, considering there was no threshold. Meanwhile, regarding the inhalation exposure for non-carcinogenic effects, the NOAEL of 6.1 mg/m^3 (based on degeneration and atrophy of the olfactory epithelium), resulting from mid-term and long-term toxicity tests on rats, was adjusted according to the test conditions, to obtain the exposure of 1.2 mg/m^3 and divided by 10 due to the short test periods. The outcome of 0.12 mg/m^3 was identified as the 'non-toxic level*' of the substance. Considering there was no threshold for the carcinogenicity, the substance's unit risk could not be identified.

With regard to the oral exposure to the substance, the absence of information on the exposure levels did not allow the health risk assessment. In addition, the MOE of 1,800 was derived from the 'non-toxic level*' of 0.21 mg/kg/day and the oral exposure level of 0.0012 μg/kg/day, estimated from the reported maximum concentrations in FY 1999 on public water bodies and freshwater, and after the division by a factor of 10 to convert animal data to human data and further by 10 to take into account the carcinogenic effects. Meanwhile, the excess incidence rate of the carcinogenic properties of the substance was calculated to be 8.4×10^{-6} from the slope factor and the oral exposure level of 0.0012μg/kg/day. As exposure to the substance in the environment through diet is limited, the MOE and the excess incidence rate would not change significantly even when this exposure is included. Therefore, collection of further information would be required to assess the health risk for the oral exposure to this substance.

Concerning the inhalation exposure to the substance, the predicted maximum exposure concentration in ambient air was approximately 0.059 $\mu g/m^3$. The MOE of 20 was derived from the 'non-toxic level*' of 0.12 mg/m^3 and the maximum exposure concentration, and after the division by a factor of 10 to convert animal data to human data and further divided by a factor of 10 to take into account the carcinogenic effects. The atmospheric maximum concentration in the high discharging plants area was 0.018 $\mu g/m^3$(annual mean), based on the emissions into the atmosphere reported in FY 2012 under the PRTR Law. The MOE of 67 was derived from this maximum level. Therefore, collection of information would be required to assess health the 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			Species	Endpoint	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	'Non-toxic level*'	0.21	mg/kg/day	Rat	Liver weight increase, forestomach hyperplasia	Drinking water	— μg/kg/day	MOE	—	×	(▲)
								Excess incidence rate	—	×	
	Slope factor	7	$(mg/kg/day)^{-1}$	Rat	Tumors at multiple sites	Groundwater	— μg/kg/day	MOE	—	×	
								Excess incidence rate	—	×	
Inhalation	'Non-toxic level*'	18	mg/m^3	Rat	Degeneration and atrophy of the olfactory epithelium	Ambient air	0.059 $μg/m^3$	MOE	20	▲	▲
								Excess incidence rate	—	×	
	Unit risk	—	$(μg/m^3)^{-1}$			Indoor air	— $μg/m^3$	MOE	—	×	×
								Excess incidence 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.

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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 101,000 μg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*; a 48-h EC_{50} of 4,130 μg/L for swimming inhibition in the crustacean *Ceriodaphnia* cf. *dubia*, which belongs to the same genus as *Ceriodaphnia dubia* (water flea); and a 96-h LC_{50} of 50,800 μg/L for the fish species *Pimephales promelas* (fathead minnow). Accordingly, based on these acute toxicity values and an assessment factor of 100, a PNEC of 41 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 12,800 μg/L for growth inhibition in the in the green alga *P. subcapitata*, and a 21-d NOEC of 4,500 μg/L for reproductive inhibition in the in the crustacean *Daphnia magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 45 μg/L was obtained.

The value of 41 μg/L obtained from the acute toxicity to the crustacean was used as the PNEC for this substance.

The PEC of this substance could not be obtained. As such, a judgment on ecological risk could not be made. However, past data yield values of 0.03 μg/L for public freshwater bodies and around 0.01 μg/L for seawater, resulting in a ratio to PNEC of less than 0.001. Accordingly, the need to collect further data on this substance is considered to be minimal 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	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)			
Crustacean *Ceriodaphnia* cf. *dubia*	Acute	EC_{50} swimming inhibition	100	41	Freshwater	—	—	×	○
					Seawater	—	—		

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Further information collection would be required for risk characterization.	（▲）
	Inhalation exposure	Collection of information 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.