

3	CAS No.: 100-44-7	Substance: Benzyl chloride
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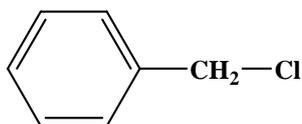
Chemical Substances Control Law Reference No.: 3-102

PRTR Law Cabinet Order No.: 1-297

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

Structural Formula:

Molecular Weight: 126.58



### 1. General information

The aqueous solubility of this substance is 493 mg/L (20°C), and the partition coefficient (1-octanol / water) (log Kow) is 2.30. The vapor pressure is 1.30 mmHg (= 1.73 Pa) (25°C). The biodegradability of the substance is good.

This substance is 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). Its uses and release sources are as a synthetic raw material -- for dyes (quinoline red, alizarin yellow-A), synthetic resins, perfumes, pyrogallol and isoquinoline -- and other uses (gasoline gum inhibitor). Import volume in 2003 was estimated at 11,500 tons.

### 2. Exposure assessment

Total release to the environment in FY2003 under the PRTR Law came to 0.36 tons. Most of this quantity was reported; the estimated release outside notification was 0.0001 tons. Release to the atmosphere accounted for a large part of the reported quantity. Chemical Industry accounted for large quantities of the reported release into both the atmosphere and public water bodies.

When estimated release outside notification are included, release to the atmosphere accounted for the greatest quantity of release to the environment. The distribution into each environmental medium predicted by means of a multimedia model was 77.9% for the atmosphere and 20.4% for water bodies.

The predicted maximum exposure concentration for inhalation exposure to human beings was approximately 0.0081 μg/m<sup>3</sup>. Moreover, when data for a limited region (Kawasaki City) were used, the predicted maximum value was reported to be approximately 0.1 μg/m<sup>3</sup>. The predicted maximum oral exposure based on groundwater and food data was estimated to be less than 0.004 μg/kg/day.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be approximately 0.05 μg/L for freshwater and less than 0.05 μg/L for seawater public water bodies.

### 3. Initial assessment of health risk

This substance is corrosive to the eyes, and even brief exposure to vapor may result in slight irritation of the eyes, skin and respiratory tract. If inhaled, it may cause a burning sensation, coughing, nausea, headache, shortness of breath and dizziness. If taken orally, it may cause abdominal pains, diarrhea, vomiting and a burning sensation. If ingested in large quantities, it may cause pulmonary edema, paralysis of the extremities, unconsciousness and so on, or even death.

Although it has been reported that cancer has been detected in laboratory animals and in workers subjected to compound exposure to α-chlorinated toluenes and benzoyl chloride (which contain in this substance), the carcinogenicity in humans in the case of exposure to this substance alone cannot be determined. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

As the level at which no adverse effect, etc. was observed, used to estimate the margin of exposure (MOE), a no observed adverse effect level (NOAEL) of 15 mg/kg/day (thyroid degeneration, hyperplasia of the lung), obtained from rat medium- and long-term toxicity testings, was obtained for oral exposure. This value was corrected for the

exposure circumstances to establish a value of 6.4 mg/kg/day. For inhalation exposure, a value of 11 mg/m<sup>3</sup> was established by correcting the NOAEL of 62 mg/m<sup>3</sup> (increased liver and spleen weight), obtained from rat and guinea pig medium- and long-term toxicity testings, to match the exposure circumstances. As the testing period was short, the value was divided by 10 to establish a value of 1.1 mg/m<sup>3</sup>.

With regard to oral exposure, the predicted maximum exposure when postulating intake of groundwater and food was less than 0.004 µg/kg/day. As the 'Non-toxic level' of 6.4 mg/kg/day and the predicted maximum exposure were established by means of animal testing, the value was divided by 10 and, out of consideration for carcinogenicity, the value was divided by 10 again to derive an MOE that exceeded 16,000. Accordingly, assessment of the environmental risk from oral exposure to this substance is thought to be unnecessary at this time.

With regard to inhalation exposure, the predicted maximum exposure concentration in ambient air was estimated at approximately 0.0081 µg/m<sup>3</sup>. The MOE derived in the same manner from the 'Non-toxic level' of 1.1 mg/m<sup>3</sup> and the predicted maximum exposure concentration was 1,400. Moreover, when ambient air data that have been reported for local areas were used to make estimates for reference purposes, the predicted maximum value was estimated at 0.1 mg/m<sup>3</sup>, and the MOE was 110. Accordingly, there is thought to be no need at this time for assessment of the health risk with regard to inhalation exposure to the substance in the ambient air. However, when local data were used, the MOE was approximately 1/10 the calculated value, near the value for which efforts to gather more data are judged to be needed. Accordingly, the release trends under the PRTR Law should be monitored, and a study should be conducted to assess the need for determination of the exposure concentration.

Exposure path	Knowledge of toxicity			Exposure assessment		Result of risk assessment			Judgment
	Guidelines for risk assessment	Animal	Impact assessment guideline (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	No observed adverse effect level 46 mg/kg/day	Rat	Thyroid degeneration, hyperplasia of the lung	Drinking water / food	— µg/kg/day	MOE	—	×	○
				Groundwater / food	< 0.004 µg/kg/day	MOE	> 16,000	○	
Inhalation	No observed adverse effect level 1.1 mg/m <sup>3</sup>	Rat Guinea pig	Increased liver and spleen weight	Ambient air	0.0081 µg/m <sup>3</sup>	MOE	1,400	○	○
				Indoor air	— µg/m <sup>3</sup>	MOE	—	×	×

#### 4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 72-hour EC<sub>50</sub> growth inhibition value of 19,300 µg/L was found for the algae *Pseudokirchneriella subcapitata*, a 96-hour LC<sub>50</sub> immobilization value of 140 µg/L was found for the crustacea *Penaeus setiferus* (prawn), and a 96-hour LC<sub>50</sub> value of 1,900 µg/L was found for the fish *Oryzias latipes* (medaka). Accordingly, an assessment factor of 100 was used, and a predicted no effect concentration (PNEC) of 1.4 µg/L was obtained based on the acute toxicity values. With regard to chronic toxicity, reliable information of a 72-hour no observed effect concentration (NOEC) growth inhibition value of 10,000 µg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 100 µg/L was found for the crustacea *D. magna* (water flea). Accordingly, an assessment factor of 100 was used, and a PNEC value of 1 µg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 1 µg/L obtained from the chronic toxicity for the crustacean was used.

The PEC/PNEC ratio was 0.05 for freshwater bodies and less than 0.05 for seawater bodies. 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	Result of assessment
Species	Acute / chronic	Endpoint			Water body	Predicted environmental concentration PEC (µg/L)		
Crustacea	Chronic	NOEC reproduction	100	1	Freshwater	0.05	0.05	○
					Seawater	< 0.05	< 0.05	

## 5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Assessment is thought to be unnecessary at this time.	○
	Inhalation exposure	Assessment with regard to the ambient air is thought to be unnecessary at this time.	○
Ecological risk	No need of further work.		○

[Risk judgments] ○: No need of further work ▲: Requiring information collection  
 ■: Candidates for further work ×: Impossible of risk characterization