1 4	CAS No.: 71-36-3	Substance: 1-butanol

Chemical Substances Control Law Reference No.: 2-3049 (as butyl alcohol)

PRTR Law Cabinet Order No.:

Molecular Formula: $C_4H_{10}O$ Structural Formula:

Molecular Weight: 74.12

$$H_3C—CH_2—CH_2—CH_2—OH$$

1. General information

The aqueous solubility of this substance is 6.32 x 10^4 mg/L (25°C), and the partition coefficient (1-octanol / water) (log Kow) is 0.88. The vapor pressure is 6.70 mmHg (= 893 Pa) (25°C). Degradability is 66% by BOD degradation rate. The substance does not have hydrolyzable groups.

The major applications for this substance are as a paint solvent (rosin, shellac, dammar, ester gum, copal, cellulose paint), as a raw material for butyl acetate, as a stabilizer, for use in alcohol refining, as fruit essence, as a raw material for dibutyl phthalate (DBP) (plasticizer), for use in pharmaceuticals, for MEK, and as butyl acrylate. Domestic production in 2003 came to 518,648 tons (as synthetic butanol). Export and import quantities are 47,287 tons and 8,611 tons, respectively.

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2. Exposure assessment

As 1-butanol is not 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), release and transfer quantities could not be obtained. When predictions of distribution ratios by medium were made using the Mackay-Type Level III Fugacity Model, in the event of equal release to the atmosphere, water and soil, the distribution ratio was highest for water and soil.

The predicted maximum exposure concentration for inhalation exposure to human beings was approximately 1.06 μg/m^3. Based on data for indoor air, the value was 72.8 μg/m^3. The predicted maximum oral exposure was estimated to be less than 0.002 μg/kg/day. Because the log Kow for this substance is low at 0.88 and bioconcentration is also predicted to be low, exposure from environmental media via the food chain is assumed to be low.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was approximately 1 μg/L for freshwater and approximately 0.22 μg/L for seawater public water bodies.

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3. Initial assessment of health risk

Exposure to vapor containing this substance may result in irritation of the eyes and respiratory tract. If inhaled, it may cause coughing, dizziness, drowsiness and headache. If taken orally, it may cause abdominal pain and vomiting. Contact with the skin may result in dryness and roughness. Contact with the eyes may result in blurred vision, a burning sensation, lacrimation, photophobia and damage to the cornea. In addition, even brief exposure may affect the central nervous system, and in high concentrations it may cause lowering of consciousness.

There is insufficient information regarding the carcinogenicity of the substance, and it is not possible to make a judgment as to whether it causes cancer in humans. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

As the 'Non-toxic level' was observed, used to estimate the margin of exposure (MOE), a no observed adverse effect level (NOAEL) of 125 mg/kg/day (decrease in locomotor activity and decreased activity) based on rat medium- and long-term toxicity testings was obtained. As the test period was short, this value was divided by 10 to establish a value of 13 mg/kg/day. In the case of inhalation exposure, the NOAEL of 150 mg/m^3 (impaired motor coordination)

obtained from rat medium- and long-term toxicity testings was corrected to match the exposure circumstances to arrive at a value of 27 mg/m^3. As the test period was short, this value was divided by 10 to establish a value of 2.7 mg/m^3.

With regard to oral exposure, when intake of groundwater was postulated, the maximum predicted exposure was less than 0.002 μg/kg/day. As the 'Non-toxic level' of 13 mg/kg/day and the maximum predicted exposure were established by means of animal testing, the value was divided by 10 to derive an MOE exceeding 650,000. Moreover, exposure originating in the environment due to the intake of food was estimated to be minor, and it is thought that adding this exposure would not greatly affect the MOE. Accordingly, assessment of the health 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 approximately 1.1 μg/m^3. Judging from the 'Non-toxic level' of 2.7 mg/m^3 and the predicted maximum exposure concentration, the MOE derived in the same manner was 250. Moreover, with regard to the concentration in indoor air, an assessment performed for reference purposes using the concentration in indoor air in reports using data for local regions arrived at a predicted maximum value of approximately 73 μg/m^3, and the MOE was 3.7. Accordingly, while 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, with regard to inhalation exposure to indoor air, the MOE (albeit based on data for local regions) was 3.7, and so this substance is thought to be a candidate for detailed assessment.

Knowledge of toxicity				Exposure assessment			Result of risk assessment			Judgment
Exposure path	Guidelines for risk assessment	Animal	Impact assessment guideline (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration					
Oral	No observed adverse effect level 13 mg/kg/day	Rat	Decrease in locomotor activity and decreased activity	Drinking water	–	μg/kg/day	MOE	–	×	○
				Groundwater	< 0.002	μg/kg/day	MOE	> 650,000	○	
Inhalation	No observed adverse effect level 2.7 mg/m^3	Rat	Impaired motor coordination	Ambient air	1.1	μg/m^3	MOE	250	○	○
				Indoor air	73	μg/m^3	MOE	3.7	■	■

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4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 72-hour EC_{50} growth inhibition value exceeding 1,000,000 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 48-hour EC_{50} immobilization value exceeding 1,000,000 μg/L was found for the crustacea *Daphnia magna* (water flea), a 96-hour LC_{50} value exceeding 100,000 μg/L was found for the fish *Oryzias latipes* (medaka), and a 48-hour LC_{50} value of 1,100,000 μg/L was found for the protozoa *Spirostmum ambiguum*. Accordingly, an assessment factor of 100 was used, and a predicted no effect concentration (PNEC) of 1,000 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 180,000 μg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 4,100 μg/L was found for the crustacea *D. magna*. Accordingly, an assessment factor of 100 was used, and a PNEC value of 41 μg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 41 μg/L obtained from the chronic toxicity for the crustacea was used.

The PEC/PNEC ratio was 0.02 for freshwater and 0.005 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	41	Freshwater	1	0.02	○
					Seawater	0.22	0.005	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Assessment is thought to be unnecessary at this time.	○
	Inhalation exposure	Although there is thought to be no need at this time for assessment of inhalation exposure to the substance in the ambient air, this substance is thought to be a candidate for detailed assessment in terms of inhalation exposure to indoor air.	○ | ■
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