14	CAS No.: 75-65-0	Substance: 2-Methylpropane-2-ol

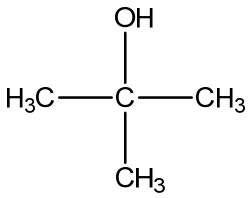
Chemical Substances Control Law Reference No.: 2-3049 (Butyl alcohol)

PRTR Law Cabinet Order No.:

Molecular Formula: $C_4H_{10}O$

Molecular Weight: 74.12

Structural Formula:



1. General information

This substance is freely miscible with water, the partition coefficient (1-octanol/water) (log K_{ow}) is 0.317 (22.5°C, pH=6.8–7.3), and the vapor pressure is 41.4 mmHg (=5.52×10^3 Pa) (25°C). Biodegradability (aerobic degradation) is judged to be difficult, and bioaccumulation is thought to be nonexistent or low. Furthermore, its half-life for hydrolysis is more than one year.

The main uses of this substance are as an organic synthesis raw material, as a solvent, as a medicated product additive (in medicated soaps and cosmetics, etc.), and as a food additive (ingredient for flavors and manufacturing).

The production and import quantity as butyl alcohol in fiscal 2014 was less than 200,000 t.

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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 using a Mackay-type level III fugacity model indicate that if equal quantities are released to the atmosphere, water bodies, and soil, the proportion distributed to water bodies would be largest.

Data for setting the maximum expected concentration of exposure to humans via inhalation could not be obtained. Further, past data for the ambient atmosphere generally indicated 0.20 μg/m^3, while that for indoor air was around 7.3 μg/m^3. The predicted maximum oral exposure was estimated to be around 0.092 μg/kg/day when calculated from data for public freshwater bodies. 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, was reported to be around 2.3 μg/L for public freshwater bodies and around 1.7 μg/L for seawater.

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3. Initial assessment of health risk

This substance is irritating to the eyes, and causes redness and pain. It may cause effects on the central nervous system. The level of consciousness could be lowered, if exposed to the substance at high concentrations. The substance causes dizziness, drowsiness, nausea, vomiting and headache, if inhaled or ingested. Contact with the skin causes redness.

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 for oral exposure of 90 mg/kg/day (based on inhibition of body weight gain), determined from long-term toxicity tests in rats, was divided by a factor of 10 to account for uncertainty in using a LOAEL. The calculated value of 9.0 mg/kg/day was deemed to be the lowest reliable dose and was identified as the

'non-toxic level*' for oral exposure.

The NOAEL for inhalation exposure of 542 ppm (based on anemia in rats, inhibition of body weight gain in mice and increase in relative weight of the liver in both species), determined from medium-term toxicity tests in rats and mice, was adjusted according to exposure conditions to obtain 96.8 ppm (293 mg/m^3), and subsequently divided by a factor of 10 to account for extrapolation from sub-chronic to chronic exposure. The obtained value of 29 mg/m^3 was deemed to be the lowest reliable concentration and was identified as the 'non-toxic level*' of the substance for inhalation exposure.

With regard to oral exposure, assuming the substance is absorbed via public freshwater bodies, the predicted maximum exposure level would be 0.092 μg/kg/day, approximately. The MOE (Margin of Exposure) would be 9,800, when calculated from the predicted maximum exposure level and the 'non-toxic level*'of 9.0 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Since exposure to the substance in environmental media via food is presumed to be limited, including the concentration in the calculation would not change the MOE significantly. 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 lack of identified exposure concentrations, the health risk could not be assessed. The maximum exposure concentration in ambient air as reported in 1995 was 0.20 μg/m^3, while the one for indoor air reported in 2004 was 7.3 μg/m^3, approximately. The MOEs would be 15,000 for ambient air and 400 for indoor air, when calculated from the respective maximum exposure concentrations and the 'non-toxic level*' of 29 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Therefore, collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air and indoor 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*' 9.0 mg/kg/day	Rats	Inhibition of body weight gain	Drinking water	— μg/kg/day	MOE	—	—	○
				Public Freshwater bodies	0.092 μg/kg/day	MOE	9,800	○	
Inhalation	'Non-toxic level*' 29 mg/m^3	Rats	Anemia and increase in relative weight of the liver.	Ambient air	— μg/m^3	MOE	—	×	(○)
		Mice	Inhibition of body weight gain and increase in relative weight of the liver.	Indoor air	— μg/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.

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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} of more than 110,000

μg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, a 48-h EC_{50} of more than 110,000 μg/L for immobilization in the crustacean *Daphnia magna*, a 96-h LC_{50} of more than 120,000 μg/L for the fish species *Oryzias latipes* (medaka), and a 48-h of LC_{50} 2,450,000 μg/L for the African clawed crab *Xenopus laevis*. A PNEC value could not be set based on these acute toxicity values because they are values obtained from limit tests that investigated the presence of effects at a designated concentration. This does not apply to other organisms.

With regard to chronic toxicity, the following reliable data was obtained: a 72-h NOEC of 110,000 μg/L for the green algae *P. subcapitata*. A PNEC value could not be set based on this chronic toxicity value because this value was obtained from a limit test that investigated the presence of effects at a designated concentration.

A PNEC could not be set for this substance because the toxicity values that can be used were obtained from limit tests that investigated the presence of effects at a designated concentration. However, if the lowest chronic toxicity value of 110,000 μg/L obtained for the algae is divided by an assessment factor of 100, the provisional PNEC value becomes 1,100 μg/L.

The PEC/provisional PNEC ratio is smaller than 0.1 for both freshwater bodies and 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	Judgment based on PEC/PNEC ratio	Assessment result
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)			
—	—	—	—	—	Freshwater	2.3	—	×	○
					Seawater	1.7	—		

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work at present.	○
	Inhalation exposure	Although risk to human health could not be confirmed, collection of further information would not be 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.