4	CAS No.: 78-83-1	Substance: Isobutyl alcohol

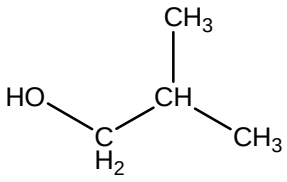
Chemical Substances Control Law Reference No.: 2-3049 (butyl alcohol)

PRTR Law Cabinet Order No.:

Molecular Formula: $C_4H_{10}O$

Molecular Weight: 74.12

Structural Formula:



1. General information

The aqueous solubility of this substance is 8.1×10^4 mg/1,000 g (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 0.76, and the vapor pressure is 10.4 mmHg (=1.39×10^3 Pa) (25°C). Biodegradability (aerobic degradation) is judged to be good. The substance does not have any hydrolyzable groups.

The main uses of this substance are as an organic synthesis solvent, a paint stripper, and a raw material for *i*-Butyl methacrylate. As butyl alcohol, the production and import quantity in fiscal 2010 was 200,000 t.

---

2. Exposure assessment

Because this substance is not classified 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), release and transfer quantities could not be obtained. The estimated release of this substance to the atmosphere from factories, based on volatile organic compound (VOC) inventories, was 46 t in fiscal 2010. Predictions of proportions distributed to individual media according to a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportions distributed to soil and water bodies would be greater.

The maximum expected concentration of exposure to humans via inhalation was around 0.74 μg/m^3 for the general environmental atmosphere and around 12 μg/m^3 for indoor air. The maximum expected oral exposure was estimated to be around 0.011 μg/kg/day on the basis of calculations from data for public freshwater bodies. The risk of exposure to this substance by intake from an environmental medium via food is considered slight, based on estimates of oral exposure obtained by using estimated concentrations in fish species.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.27 μg/L for public freshwater bodies and around 0.29 μg/L for seawater.

3.Initial assessment of health risk

This substance may cause irritation to skin, with significant irritation especially to eyes. Chemical pneumonia may be caused if liquid of the substance is swallowed to lungs. Symptoms of poisoning by its inhalation include headache, dizziness and lethargy, while those by ingestion also include nausea, diarrhea and vomiting. Contact of the substance with eyes may cause redness and pain, while its contact with skin may cause redness, pain and dry skin. Its lethal dose for human is reported to be 428 mg/kg.

As sufficient information was not available to evaluate carcinogenic potential of the substance, an initial assessment was conducted on the basis of information on its non-carcinogenic effects.

With regard to oral exposure to the substance, a NOAEL of 297 mg/kg/day (for increased kidney weight) obtained from its mid-term and long-term toxicity tests on rats was identified to be the reliable lowest dose as its ‘non-toxic level*’. With regard to inhalation exposure to the substance, a NOAEL of 1,044 ppm (for increased

red blood cells, hemoglobin levels and hematocrit levels) for female animals obtained from its mid-term and long-term toxicity tests on rats was adjusted for their durations to provide 186 ppm (560 mg/m^3) for its intermittent to continuous exposure and divided by a factor of 10 due to their short test periods. 56 mg/m^3 was identified to be the reliable lowest dose as its 'non-toxic level*'.

As for its oral exposure, its maximum exposure concentration was predicted to be approximately 0.011 μg/kg/day, when its intakes through freshwater from public water bodies were assumed. The MOE (Margin of Exposure) would be 2,700,000 when calculated from the substance's 'non-toxic level*' of 297 mg/kg/day and the maximum exposure concentration predicted from animal experiments and divided by a factor of 10 to convert animal data to human. As exposure to the substance in the environment through food intakes would be limited, the MOE would not change significantly even when this exposure was included. Therefore, no further action would be required at this moment to assess its health risk from oral exposure.

With regard to inhalation exposure to the substance, the maximum exposure concentration in the ambient air was predicted to be about 0.74 μg/m^3. The MOE would be 7,600 when calculated from the substance's 'non-toxic level*' of 56 mg/m^3 and the maximum exposure concentration predicted from animal experiments and divided by a factor of 10 to convert animal data to human. As for concentrations in the indoor air, the MOE would be 470 when the maximum exposure concentration was predicted to be approximately 12 μg/m^3. Therefore, no further action would be required at this moment to assess health risk from its inhalation both in the ambient air and in the 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*' 297 mg/kg/day	Rat	Increased kidney weight	Drinking water	— μg/kg/day	MOE	—	×	○
				Freshwater	0.011 μg/kg/day	MOE	2,700,000	○	
Inhalation	'Non-toxic level*' 56 mg/m^3	Rat	Increased red blood cells, hemoglobin levels and hematocrit levels	Ambient air	0.74 μg/m^3	MOE	7,600	○	○
				Indoor air	12 μg/m^3	MOE	470	○	○

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

With regard to acute toxicity, the following reliable data were obtained: a 48-h EC_{50} of 2,300,000 μg/L for growth inhibition in the green alga *Desmodesmus subspicatus*, a 96-h LC_{50} of 949,000 μg/L for the crustacean *Orconectes immunis* (North American freshwater crayfish), a 96-h LC_{50} of 1,330,000 μg/L for the fish species *Oncorhynchus mykiss* (rainbow trout), and a 48-h LC_{50} of 2,090,000 μg/L for the midge *Tanytarsus dissimilis*. Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 9,490 μg/L was obtained.

With regard to chronic toxicity, a 21-d NOEC of 4,000 μg/L for reproductive inhibition in the crustacean *Daphnia magna* was obtained as a reliable data. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 40 μg/L was obtained.

The value of 40 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.007 for both freshwater bodies and seawater. Accordingly, further work is considered unnecessary at this time.

Hazard assessment (basis for PNEC)			Assessment factor	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 *Daphnia magna*	Chronic	NOEC Reproductive inhibition	100	40	Freshwater	0.27	0.007	○	○
					Seawater	0.29	0.007		

---

5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	No need for further work.	○
Ecological risk	No need of further work at present.		○

［Risk judgments］ ○: No need for further work ▲: Requiring information collection

■: Candidates for further work ×: Impossibility of risk characterization

（○）: Though a risk characterization cannot be determined, there would be little necessity of collecting information.

（▲）: Further information collection would be required for risk characterization.