5 CAS No.: 95-16-9 Substance: Benzothiazole

Chemical Substances Control Law Reference No.: 5-3426

PRTR Law Cabinet Order No.:

Molecular Formula: C₇H₅NS Structural formula:

Molecular Weight: 135.19



1. General information

The aqueous solubility of this substance is 4.30×10^3 mg/L (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 2.01, and the vapor pressure is 0.074 mmHg (=9.9 Pa) (25°C, calculated value). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and bioaccumulation is thought to be nonexistent or low.

The main use of benzothiazoles is addition to rubber as a vulcanizer and antioxidant. The substance was removed from the Class 2 Designated Chemical Substance list as a result of the revision of substances regulated by the Law Concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law) enacted on October 1, 2009. The production and import category under the PRTR Law was 1 to <100 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 distribution by medium using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to soil would be greater.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, is around 0.45 μ g/L for public freshwater bodies and generally less than 0.087 μ g/L for seawater.

3. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC₅₀ of more than 45,800 μ g/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*, a 48-h EC₅₀ of 19,000 μ g/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC₅₀ of 39,000 μ g/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment coefficient of 100, a predicted no effect concentration (PNEC) of 190 μ g/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 8,450 μ g/L for growth inhibition in the green algae *P. subcapitata* and a 21-d NOEC of 1,500 μ g/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment coefficient of 100, a predicted no effect concentration (PNEC) of 15 μ g/L was obtained. The value of 15 μ g/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.03 for freshwater bodies and less than 0.006 for seawater. Accordingly, further work is thought to be unnecessary at this time.

Hazard assessment (basis for PNEC)				Predicted no	Exposure assessment			Judgment	
Species	Acute/ chronic	End point	Assessment	effect concentration PNEC (µg/L)	Water body	Predicted environmental concentration PEC (µg/L)	PEC/ PNEC ratio	based on PEC/PNEC ratio	Assessment
Crustacean		NOEC			Freshwater	0.45	0.03		
Daphnia magna	Chronic Reproductive inhibition	100	15	Seawater	<0.087	<0.006	0	0	

4. Conclusions

	Conclusions	Judgment					
Ecological risk	No need of further work at present	0					
[Risk judgment	○: No need for further work						
■: Candidates for further work ×: Impossibility of risk characterization							
	(O): Though a risk characterization cannot be determined, there would be l	ittle necessity of					
	collecting information.						
	(A) : Further information collection would be required for risk characterization.						