

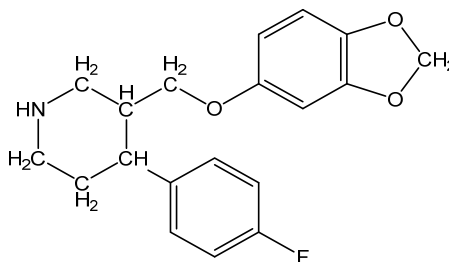
Chemical Substances Control Law Reference No.:

PRTR Law Cabinet Order No. :

Structural Formula:

Molecular Formula: C₁₉H₂₀FNO₃

Molecular Weight: 329.37



1. General information

The aqueous solubilities of this substance are 7.46 mg/L (25°C) (calculated value) and 17.14 mg/L (25°C) (hydrochloride, calculated value), the partition coefficients (1-octanol/water) (log K_{ow}) are 4.74 (calculated value) and 2.89 (hydrochloride, calculated value), and the vapor pressures are 6.39×10⁻⁶ Pa (calculated value) and 1.56×10⁻¹⁰ Pa (hydrochloride, calculated value). In terms of biodegradability (aerobic degradation), this substance is reported to not break down (hydrochloride 1/2 hydrate). In addition, this substance is stable towards hydrolysis (hydrochloride 1/2 hydrate) (25°C, half-life: more than 1 year).

The main use of this substance's hydrochloride hydrate is as a selective reuptake inhibitor for serotonin. The production quantity of this substance calculated based on production of paroxetine hydrochloride hydrate was 1.4 t in 2019 and the import quantity was 0.29 t.

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

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.0029 µg/L for public freshwater bodies, and generally less than 0.00065 µg/L for seawater.

3. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 48-h EC₅₀ of 130 µg/L for growth inhibition in the green alga species *Raphidocelis subcapitata*, 48-h LC₅₀ of 580 µg/L for the crustacean species *Ceriodaphnia dubia*, and a 96-h LC₅₀ of 5,120 µg/L for African clawed frog *Xenopus laevis* embryos. Accordingly, based on these acute toxicity values and an assessment factor of 1,000, a predicted no effect concentration (PNEC) of 0.13 µg/L was obtained.

With regard to chronic toxicity, the following reliable datum was obtained: a 7–8-d NOEC of 220 µg/L for reproductive inhibition in the crustacean species *C. dubia*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 2.2 µg/L was obtained.

The value of 0.13 µg/L obtained from the acute toxicity to the green alga species was used as the PNEC for this substance

The PEC/PNEC ratio is 0.02 for freshwater bodies and less than 0.005 for seawater; accordingly, further work to assess the ecological risk of this substance is considered unnecessary at this time. A comprehensive review of the above findings draws the same conclusion.

Hazard assessment (basis for PNEC)			Assessment coefficient	Predicted no effect concentration PNEC (µg/L)	Exposure assessment		PEC/PNEC ratio	Comprehensive judgment
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (µg/L)		
Green algae	Acute	EC ₅₀ Growth inhibition	1,000	0.13	Freshwater	0.0029	0.02	○
					Seawater	<0.00065	<0.005	

4. Conclusions

	Conclusions	Judgment
Ecological risk	No need for further work	○

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