| 9 | CAS No. 55-63-0 | Substance: Nitroglycerine |
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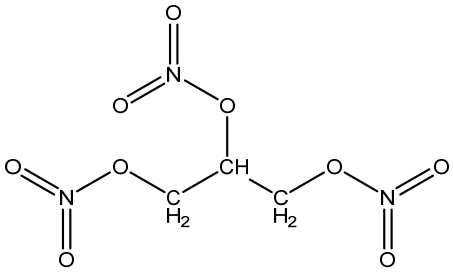
Chemical Substances Control Law Reference No.: 2-1574

PRTR Law Cabinet Order No.: 1-313

Molecular Formula: $C_3H_5N_3O_9$

Molecular Weight: 227.09

Structural Formula:



**1. General information**

The aqueous solubility of this substance is $1.3\times10^3$ mg/1000g (19°C), the partition coefficient (1-octanol/water) (log $K_{ow}$) is 1.62, and the vapor pressure is $4\times10^{-4}$ mmHg (=0.05 Pa) (25°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 53.6%, while half-lives for hydrolysis of 1–10 years (25°C, pH=8–7) and 2.6–26 years (18°C, pH=8–7) have been calculated.

This substance is classified as a Class 1 Designated Chemical Substance under the PRTR Law. The main use of this substance is as a key ingredient for smokeless powder. It is also used as an active ingredient in pharmaceuticals (for congestive heart failure, myocardial infarction, and angina attacks). The production and import quantity in fiscal 2017 was not disclosed because the number of reporting businesses was not more than two. The production and import category under the PRTR Law is more than 100 t.

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**2. Exposure assessment**

Total release to the environment in fiscal 2017 under the PRTR Law was 0.60 t, and all releases were reported. All reported releases were to the atmosphere, and 0.009 t was transferred to waste materials. The chemical industry was the sole reporter of releases. A multimedia model used to predict the proportions distributed to individual media in the environment indicates that in regions where the largest quantities were estimated to have been released to the environment overall or the atmosphere in particular, the predicted proportion distributed to soil was 77.8% and that to water bodies was 18.6%.

The maximum expected concentration of exposure to humans via inhalation could not be determined because ambient atmospheric and indoor air quality data could not be obtained. The mean annual value for the atmospheric concentration in fiscal 2017 was calculated by use of a plume-puff model on the basis of releases to the atmosphere reported according to the PRTR Law; this model predicts a maximum level of 0.16 μg/$m^3$ .

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. However, no releases to public freshwater bodies were reported in in fiscal 2017 under the PRTR Law; accordingly, this substance's concentration in public water bodies is thought to be low. The risk of exposure to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on the basis of its physicochemical properties.

Estimates for exposure to aquatic organisms based on measured data could not be carried out. No releases to public freshwater bodies were reported in fiscal 2017 under the PRTR Law; accordingly, this substance's concentration in public water bodies is thought to be low.

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**3. Initial assessment of health risk**

This substance is irritating to the eyes. Inhalation of the substance causes headache, nausea, flushing of the face and dizziness. Ingestion causes vomiting and shock or collapse, in addition to the same symptoms as inhalation. The substance on the skin may be absorbed to cause headache, nausea and some other symptoms. Contact with the eyes causes redness and pain.

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 of 0.13 mg/kg/day for oral exposure (based on cerebral vasodilation), determined from the effects observed in humans, was divided by a factor of 10 to account for uncertainty in using a LOAEL. The calculated value of 0.013 mg/kg/day was deemed to be the lowest reliable dose and was identified as the 'non-toxic level' of the substance for oral exposure. The NOAEL of 0.093 mg/m$^3$ for inhalation exposure (based on headache), determined from the effects observed in humans, was adjusted according to exposure conditions. The calculated value of 0.019 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, owing to the lack of identified exposure levels, the health risk could not be assessed. The total release of the substance to the environment was reported to be approximately 0.60 t in FY 2017 under the PRTR Law. However, the release of the substance into public water bodies was reported to be 0 t, and predictions of the multimedia fugacity model indicated that the proportion distributed to water was little. Therefore, as a comprehensive judgment, collection of further information would not be required to assess the health risk of this substance via oral exposure.

With regard to inhalation exposure, owing to the lack of identified exposure concentrations, the health risk could not be assessed. However, the MOE (Margin of Exposure) for reference would be 120, when calculated from the concentration in ambient air of 0.16 μg/m$^3$ and the 'non-toxic level' for inhalation exposure of 0.019 mg/m$^3$. This concentration was estimated as the maximum concentration (annual mean) in ambient air near the operators releasing large amount of this substance based on the releases to air reported in FY 2017 under the PRTR Law. Therefore, as a comprehensive judgment, collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air.

| Toxicity | | | | Exposure assessment | | MOE | | Comprehensive judgment |
|---|---|---|---|---|---|---|---|---|
| Exposure Path | Criteria for risk assessment | Animal | Criteria for diagnoses (endpoint) | Exposure medium | Predicted maximum exposure dose and concentration | | | |
| Oral | 'Non-toxic level' 0.013 mg/kg/day | Humans | Cerebral vasodilation | Drinking water | - μg/kg/day | MOE | - | ○ |
| | | | | Groundwater | - μg/kg/day | MOE | - | |
| Inhalation | 'Non-toxic level' 0.019 mg/m$^3$ | Humans | Headache | Ambient air | - μg/m$^3$ | MOE | - | ○ |
| | | | | 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 96-h $EC_{50}$ exceeding 1890 μg/L for growth inhibition in the alga *Raphidocelis subcapitata*, a 48-h $LC_{50}$ of 17,830 μg/L for the crustacean *Ceriodaphnia dubi*a, a 96-h $LC_{50}$ of 1670 μg/L for the fish *Lepomis macrochirus* (bluegill), and a 48-h $LC_{50}$ of 17,430 μg/L for the cnidarian *Hydra littoralis*. Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 16 μg/L was obtained

With regard to chronic toxicity, the following reliable data were obtained: a 96-h NOEC of 370 μg/L for growth inhibition in the alga *R. subcapitata*, a 7-d NOEC of 3230 μg/L for reproductive inhibition in the crustacean *C. dubia*, and a 60-d NOEC of 30 μg/L for embryo and post-hatch growth inhibition in the fish *Oncorhynchus mykiss* (rainbow trout). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a PNEC of 3 μg/L was obtained.

The value of 3 μg/L obtained from the chronic toxicity to the fish species was used as the PNEC for this substance.

Data for setting the predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained; accordingly, ecological risk assessment could not be carried out.

However, no releases to public freshwater bodies were reported in in fiscal 2017 under the PRTR Law; accordingly, this

substance's concentration in public water bodies is thought to be low. Accordingly, based on a comprehensive review of the above findings, there is little need to collect new data regarding this substance.

| 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) | | |
| Fish *Oncorhynchus mykiss* | Chronic | NOEC Growth inhibition | 10 | 3 | Freshwater | — | — | ○ |
| | | | | | Seawater | — | — | |

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**5. Conclusions**

| | Conclusions | | Judgment |
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| Health risk | Oral exposure | No need for further work. | ○ |
| | Inhalation exposure | No need for further work. | ○ |
| 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