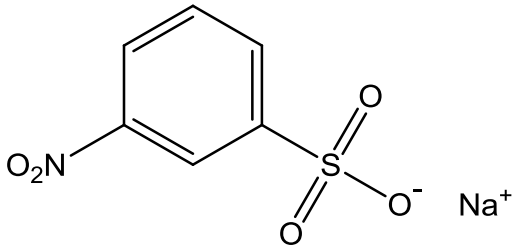
INITIAL TARGETED ASSESSMENT PROFILE

CAS No.	127-68-4
Chemical Name	Sodium 3-nitrobenzenesulfonate
Structural Formula	

SUMMARY CONCLUSIONS OF THE TARGETED ASSESSMENT

NOTE: The present assessment is targeted to address only the following endpoint(s): Human Health: acute toxicity, repeated dose toxicity and *in vitro* mutagenicity. It cannot be considered as a full SIDS Initial Assessment. Nevertheless, the conclusions for the endpoints addressed have been agreed by member countries and may be used for hazard and risk assessment. Results on other endpoints may be relevant for hazard and risk assessment but have not been addressed in the assessment.

Rationale for targeting the assessment

Under the Japanese Chemical Substances Control Law, hazard assessment of existing chemical substances via environmental exposure has been conducted. If a chemical substance is evaluated as "not biodegradable (persistent)" and "not highly bioaccumulative", at least, a 28-day repeated dose toxicity and two *in vitro* mutagenicity studies are required as screening studies for hazard evaluation regarding human health. If a chemical is evaluated as having potential of long- term toxicity for human health, the chemical is classified as a Type II Monitoring Chemical Substance. If not, the chemical is of low priority for further action. Type II Monitoring Chemical Substances undergo risk-based management; at first, annual production volumes of those substances are monitored.

Sodium 3-nitrobenzenesulfonate was evaluated as "not biodegradable (persistent)" and "moderately bioaccumulative" by the METI (Ministry of Economy, Trade and Industry, Japan). Biodegradation and bioaccumulation are not parts of the targeted assessment and therefore not presented in the ITAP. In order to determine whether this chemical is classified as a Type II monitoring chemical substance, the initial hazard assessment of sodium 3-nitrobenzenesulfonate was conducted for the repeated dose toxicity and mutagenicity by MHLW (Ministry of Health, Labour and Welfare, Japan) in September 2005.

This targeted assessment document was originally based on the material from the chemical assessment council of MHLW, and the toxicological profile was re-assessed for the OECD Cooperative Chemicals Assessment Programme.

Physical-chemical properties

Sodium 3-nitrobenzenesulfonate is a pale yellow powder at standard temperature and pressure. Melting point and boiling point are 52.30 °C and 217.50 °C, respectively. Vapour pressure is calculated to be 10.3 Pa at 25 °C by MPBPWIN. The partition coefficient between octanol and water (log K_{ow}) is calculated to be -3.13 by KOWWIN. Water solubility is calculated to be 1.0 x 10^6 mg/L at 25 °C by WSKOWWIN. It is considered that sodium ion of this chemical is dissociated from sulfonate group in water.

Human Health

No reliable information was found on the acute toxicity of sodium 3-nitrobenzenesulfonate. However, as no treatment related mortality or no clinical signs of toxicity were found up to 1000 mg/kg bw/day at the beginning of dosing in a 28-day repeated oral gavage toxicity study, it is assumed that the LD_{50} value is more than 1000

mg/kg bw. Less reliable information indicates an oral LD_{50} value of 11 g/kg bw in rats.

A repeated dose oral toxicity study in rats was conducted following Guideline for 28-Day Repeated Dose Toxicity Test in Mammalian Species (Chemical Substances Control Law of Japan). In this study, sodium 3-nitrobenzenesulfonate was administered via gavage at 0 (vehicle control: corn oil), 100, 300 or 1000 mg/kg bw/day for 28 days. Ten animals/sex (in the control and top-dose group) and 5 animals/sex (in the low and medium-dose groups) were used. There were no deaths and no treatment-related toxicological effects in either sex. As for the possibility of the methemoglobin formation, in contrast, the levels of methemoglobin at 1000 mg/kg bw/day in both sexes tended to decrease. No related changes were observed. Based on the findings, the NOAEL for this 28-day repeat dose toxicity study is considered to be 1000 mg/kg bw/day (the highest dose tested) for both sexes.

In a bacterial mutation study using four strains of *Salmonella typhimurium* and one strain of *Escherichia coli*, sodium 3-nitrobenzenesulfonate was negative with or without metabolic activation. In an *in vitro* chromosome aberration test using CHL/IU cells, sodium 3-nitrobenzenesulfonate was also negative with or without metabolic activation. Based on these results, sodium 3-nitrobenzenesulfonate is not considered to be genotoxic *in vitro*.

Agreed hazard conclusions

This chemical has a low hazard profile for the human health endpoints (repeated dose toxicity and gene mutations and chromosomal aberrations) targeted in this assessment. Toxicity studies via relevant routes of occupational exposure were not identified in this targeted assessment.

Available Exposure information

Production volume and/or import volume of sodium 3-nitrobenzenesulfonate in Japan (sponsor country) was between 100 and 1,000 tonnes in 2007. Production and/or import volume of sodium 3-nitrobenzenesulfonate in the United States was between 1 million and 10 million pounds (454,000 - 4,540,000 tonnes) during 2006 according to the U.S. Inventory Update Reporting. Information of the production volume in other areas was not obtained.

Sodium 3-nitrobenzenesulfonate is used as a dye intermediate, dyeing aid and plating remover in Japan. Dermal and inhalation exposure of workers is expected.