201-16248

Oxirane, reaction products with ammonia, distillation residue

CAS Number 68953-70-S

USEPA HPV Challenge Program Submission

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Submitted by:

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I. Introduction

Huntsman Petrochemical Corporation and INEOS Oxide, a division of INEOS Americas, LLC have voluntarily committed to develop screening level health effects data, environmental fate and effect data, and physical chemical test data for the distillation residue from the reaction of oxirane with ammonia (CAS # 68953-70-8) under the Environmental Protection Agency's High Production Volume Challenge Program.

This organic amine stream is the resulting distillation residue from alkanolamines production. In this process, ethylene oxide is reacted with ammonia to form mono-, di- and tri- ethanolamines. These fractions are removed by distillation. The remaining distillation residue is CAS# 68953-70-8. This material typically contains at least 80% TEA, less than 1% DEA, with the remainder as higher boiling amine reaction products.

CAS# 68953-70-8 is used mainly as a concrete additive as a corrosion inhibitor for steel reinforcements. Environmental and occupational exposures are expected to be minimal.

Data Availability and Quality Summary

	Data Available	Data Adeauate	Testing Recommended
Melting point	TEA	Yes	No
Boiling point	Yes	Yes	No
Vapor Pressure	Yes	Yes	No
Partition Coefficient	TEA	Yes	No
Water Solubility	Yes	Yes	No
Stability in Water	TEA	No	No
Transport	TEA	Yes	No
Photodegradation	No	Yes	No
Biodegradation	TEA	Yes	No
Acute Toxicity to Fish	TEA	Yes	No
Acute Toxicity to Invertabrates	TEA	Yes	No
Acute Toxicity to Aquatic Plants	TEA	Yes	No
Acute Tox – oral	**Yes**	**Yes**	**No**
Acute Tox – inhalation	TEA	**Yes**	**No**
Acute Tox – dermal	Yes	**Yes**	**No**
Gene Tox – MN	Yes	**Yes**	**No**
Gene Tox *in vitro* – Ames	Yes	**Yes**	**No**
Gene Tox *in vitro* – *UDS*	Yes	**Yes**	**No**
Repeat dose- oral, dermal, inhalation	TEA	**Yes**	**No**
Reproductive toxicity	TEA	**Yes**	**No**
Developmental tox	TEA	**Yes**	**No**

II. Use of Triethanolamine Data for CAS Number 68953-70-8 Endpoints

As described above, CAS# 68953-70-8 is the distillation residue from alkanolamines production and it typically contains at least 80% triethanolamine (TEA). Because of this relatively high percentage of TEA, the toxicity of CAS# 68953-70-8 would be expected to be very similar to that of commercial TEA. This data summary and test plan includes available data on CAS# 68953-70-8, compares that data to TEA data for the same endpoints, and uses TEA data as a surrogate for other endpoints.

Endpoint	CAS# 68953-70-8	TEA
Boiling point	372 C	335 c
Vapor Pressure	<0.1 mmHg	<0.1 mmHg
Water Solubility	Miscible	Miscible
Acute Tox – oral	>5000 mg/kg	>5000 mg/kg
Acute Tox – dermal	>3000 mg/kg	>2000 mg/kg
Gene Tox ***in vivo – MN***	Negative	
- Drosophila SLRL		Negative
Gene Tox ***in vitro*** – Ames	Negative	Negative
Gene Tox ***in vitro – UDS***	Negative	Negative

III. Test Plan and Rationale

A. Physical Chemical Data

The physical/chemical data for CAS# 68953-70-s are found in material safety data sheets. The underlying data were not reviewed, but additional testing is not justified. Transport between environmental compartments has been estimated using EPA software (EPIWIN Level III). The stability of CAS# 68953-70-8 in water has not been tested, but TEA was stable in two river water samples for 7 or 10 days.

Recommended testing: None

B. Ecotoxicity

CAS# 68953-70-8 or TEA lack chromophoric functional groups for participation in photodegradation at environmentally relevant wavelengths; thus there are no photodegradation data and none are needed. Data on biodegradation of CAS# 68953-70-8 are not available; however, in reactions with mixed liquor activated sludge from a municipal wastewater treatment facility, TEA biodegrades with an estimated half-life of 0.02 to 0.1 days. (Because this study was not included in the TEA IUCLID, it is

included in the CAS# 68953-70-8 IUCLID.) Data on acute fish, invertebrate and plant toxicity for CAS# 68953-70-8 were not found, but data on TEA are available to cover this endpoint. Acute fish toxicity studies *(Carassius auratus, Lepomis macrochirus, Leuciscus idus, and Pimephales promelas)* are included in the TEA IUCLID data set; acute fish LC_{50}s are > 450 mg/l to >11,800 mg/l. An acute toxicity study of TEA to *ceriodaphnia dubia* (water flea) was not included in the TEA IUCLID, so is included in the IUCLID for CAS# 68953-70-8; the EC_{50} for 48 hour exposure was 610 mg/l. The toxicity of TEA to *Scenedesmus subspicatus* (Green algae) was not included in the TEA IUCLID, so is included in the IUCLID for CAS# 68953-70-8; the EC_{50} for 48 hour exposure, based on decreased biomass, was 470 mg/l in a static cell multiplication inhibition test.

Recommended ecotoxicity testing: None

C. Mammalian Toxicity

Reliable acute toxicity tests are available on CAS# 68953-70-8 and TEA. CAS# 68953-70-8 is practically nontoxic following acute oral exposure in a test that meets OECD and EPA test guidelines; the LD_{50} is >5000 mg/kg. The dermal LD_{50} is >3000 mg/kg, in a test that meets OECD and EPA test guidelines. LD_{50}s for TEA were similar. No further testing is recommended.

Repeated dose testing of CAS# 68953-70-8 data are not available, but subchronic (l-3 month) studies of TEA by oral, inhalation, and dermal exposure are available. A one month inhalation study of TEA is included in the TEA IUCLID (p. 33); exposure of rats 6 hr/d, 5 d/wk for 4 wk to an aerosol of TEA at 20, 100 and 500 mg/m^3 revealed no adverse effects except slight inflammation of mucosa of the larynx. TEA in the feed of rats for 91 days at up to 1000 mg/kg body weight (included in TEA IUCLID, p. 35) resulted in no treatment-related effects. Dermal application (studies included in TEA IUCLID, p. 37, 41) of TEA to rats at 125 to 2000 mg/kg/day for 91 days or mice at 250 to 4000 mg/kg/day for 91 days resulted in no systemic toxicity, but slight inflammation at the exposure site. No further testing is recommended.

CAS# 68953-70-8 was negative in an Ames (in vitro bacterial mutation) assay, a rat hepatocyte UDS (in vitro DNA damage and repair) assay and a micronucleus (in vivo genotoxicity) assay in mice. TEA was also negative in five Ames assays, two *Bacillus subtilis* recombination assays, two E. coli mutation assays, one *Saccharomyces cerevisae* mutation assay, two *in vitro* chromosomal aberration assays, one *in vitro* sister chromatid exchange assay, two *in vitro UDS* assays, one *in vitro* CHO cell transformation assay, and one *in vivo* sex-linked recessive lethal mutation assay in *Drosophila melanogaster*. No further testing is recommended.

TEA has been reported not to increase tumors in rats in a 2 yr drinking water study (TEA IUCLID, p. 50) or in an 18 month study in mice (TEA IUCLID, p. 51). No increase in tumors was found in mice exposed to TEA for two years at 40 or 450

mg/kg/day body weight in the feed (TEA IUCLID, p. 51). No increase in tumors was found following dermal application for 14-18 months in two separate studies (TEA IUCLID, p. 49).

No reproduction studies have been found for either CAS# 68953-70-8 or TEA; however, no toxicity to reproductive organs has been reported in any of the repeated-dose toxicity studies of TEA. Therefore, reproductive toxicity is unlikely for CAS# 68953-70-8. No further testing is recommended.

No change in maternal mortality, number of viable litters, litter size, percent survival of pups, or birth weight or weight gain of pups was found when mice were dosed with TEA by gavage at 1125 mg/kg on gestation days 6-15 and evaluated on post pat-turn day 3 (TEA IUCLID, p. 53). No increase in malformations was seen when hair dyes containing TEA (30 mg/kg/day) were applied to the skin of rats on gestation days 1, 4, 7, 10, 13, 16, and 19 (TEA IUCLID, p. 54). No further testing is recommended.

Recommended Testing: None