

201-15677

HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM

U.S. ENVIRONMENTAL PROTECTION AGENCY  
WASHINGTON, D.C. 20460

**TEST PLAN**

**For**

**2,4,8,10-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)-  
CAS No. 3806-34-6**

**Submitted to the US EPA  
BY**

# **Crompton Corporation.**

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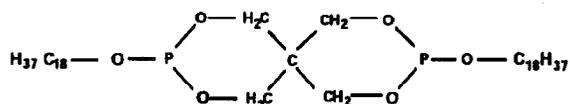
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## 1. General Information

1.1 CAS Number: 3806-34-6

1.2 Molecular Weight: 733.06

1.3 Structure and formula:  $C_{41}H_{82}O_6P_2$



## 1.4 Introduction

2,4,8,10-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- (Weston 618) is used as a color and molecular weight stabilizer for polyolefins, polyesters, elastomers, styrenics, engineering thermoplastics and adhesive formulations.

## 2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for Weston 618.

The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing on Weston 618

CAS No. <b>3806-34-6</b>	Information Available?	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
<b>Physicochemical</b>							
Melting Point	Y	N				Y	N
Boiling Point	Y				Y	Y	N
Vapour Pressure	Y				Y	Y	N
Water Solubility	Y	Y			Y	Y	N
Partition Coefficient (Kow)	Y				Y	Y	N
<b>Environmental Fate</b>							
Biodegradation	Y				Y	Y	N
Hydrolysis	N						N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
<b>Ecotoxicology</b>							
Acute Fish	Y				Y	Y	N
Acute Daphnia	Y				Y	Y	N
Acute Algae	Y				Y	Y	N
<b>Toxicology</b>							
Acute Oral	Y	N	N			Y	N
Repeat Dose toxicity	Y	N	N			Y	N
Genetic toxicity – Gene mutation	Y	N				Y	N
Genetic toxicity – Chromosome aberration	Y	Y	Y			Y	N
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

**A. Evaluation of Existing Physicochemical Data and Proposed Testing**

1. Melting Point

The melting point was reported to be between 37 - 46°C a manufacturer's MSDS.

2. Boiling Point

The boiling point was estimated to be 705°C using MPBPWIN v 1.40.

3. Vapor Pressure

The vapor pressure was estimated to be  $1.06 \times 10^{-18}$  hPa at 25°C using MPBPWIN v 1.40.

4. Water Solubility

The water solubility could not be experimentally determined because the test substance is hydrolytically unstable. The water solubility is estimated to be  $2.95 \times 10^{-12}$  mg/L at 25°C using WSKOW v 1.40.

5. Partition Coefficient

The Log Pow is estimated to be 15 using KOWWIN v 1.66.

**Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure, partition coefficient and water solubility are considered to fill these endpoints adequately.**

**B. Evaluation of Existing Environmental Fate Data and Proposed Testing**

1. Biodegradation

The biodegradability of the chemical has been estimated using Biowin v4.00 and the results indicate the chemical to not be readily biodegradable. The chemical contains no biodegradable groups, therefore no biodegradation testing is proposed.

2. Hydrolysis

A GLP study was conducted on the test substance in water, and it was determined that due to the poor solubility and hydrolytically unstable as determined during the water solubility testing, a half-life could not be determined. The Fugacity model calculated half-life was 1.44 e003 hr.

The test substance is hydrolytically unstable as determined during the water solubility testing. Therefore no additional stability test will .performed.

3. Photodegradation

The potential for photodegradation of Weston 618 has been estimated using the AOPWIN v1.90, and indicated atmospheric oxidation via OH radicals reaction with a half-life of 0.689 hours.

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted and indicates distribution mainly to sediment and, to a lesser extent, soil for emissions of 1000 kg/hr simultaneously to air water and soil compartments.

**Summary of Environmental Fate Testing: Existing data for photodegradation, hydrolysis, biodegradation and transport and distribution between environmental compartments are considered to fill these endpoints adequately.**

**C. Evaluation of Existing Ecotoxicity Data and Proposed Testing**

1. Acute Toxicity to Fish

The LC<sub>50</sub> (96 h) was estimated to be  $2.94 \times 10^{-10}$  mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

2. Acute Toxicity to Daphnia

The EC<sub>50</sub> (48 h) was estimated to be  $7.76 \times 10^{-10}$  mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

3. Acute Toxicity to Algae

The EC<sub>50</sub> (96 h) was estimated to be  $1.03 \times 10^{-9}$  mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

**Summary of Ecotoxicity Testing: Weston 618 is estimated to be toxic to the environment only at levels above its limit of solubility. No further testing is proposed.**

**D. Evaluation of Existing Human Health Effects Data and Proposed Testing**

1. Acute Oral Toxicity

The acute oral toxicity of Weston 618 is reported as LD<sub>50</sub> > 10000 mg/kg in a rat study. None of the animals showed any signs of toxicity at the maximum dose.

2. Acute Dermal Toxicity (non-SIDS endpoint)

Acute dermal toxicity was reported as LD<sub>50</sub> > 2000 mg/kg using rabbits in an OECD 402 study conducted to GLP.

3. Eye Irritation (non-SIDS endpoint)

Weston 618 was found to be non-irritating to rabbit eyes.

#### 4. Repeat Dose Toxicity

In a 90-day oral feed study conducted using rats, the observed NOAEL was > 3000 ppm. There were no significant differences between controls and the dose groups in any of the parameters studied.

#### 5. Genotoxicity

Ultranox 626 tested negative in an Ames test using *Salmonella typhimurium* strains TA97, TA98, TA100 and TA102 and *Escherichia coli* strain WP2 (PKM101) with and without metabolic activation.

In an in vivo mouse micronucleus assay (OECD 474) no genotoxic effects were observed at doses up to 2000 mg/kg (the maximum dose tested).

#### 6. Reproductive and Developmental Toxicity

An OECD 421 study will be performed to fill this end point.

**Summary of Human Health Effects Testing: All endpoints are considered to have been filled adequately, except for the reproductive/developmental toxicity endpoint. This endpoint will be filled by performing an OECD 421 study.**

### 3. Evaluation of Data for Quality and Acceptability

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

- (1) **Reliable without restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.
- (2) **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.
- (3) **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.
- (4) **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

### 4. References

- [1] US EPA, EPI Suite Software, 2000

- [2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.
- [3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5
- [4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.