

AR201-13209A

DATA SUMMARY & TEST PLAN
For
2-Hydroxy-4-n-Octoxybenzophenone

October 10, 2001

OVERVIEW

Cytec Industries Inc. and Ciba Specialty Chemicals Corporation hereby submit for review a test plan for 2-Hydroxy-4-n-Octoxybenzophenone under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of these companies to use existing data to adequately fulfill the Screening Information Set (SIDS) for environmental fate endpoints, ecotoxicity tests, and human health effects for this substance. We believe that adequate data exist to fulfill all the requirements of the HPV program without the need for additional testing.

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US EPA High Production Volume (HPV)
Chemical Challenge Program

**Data Summary
&
Test Plan**

**2-Hydroxy-4-n-Octoxybenzophenone
CAS No. 1843-05-6**

October 10, 2001

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DATA SUMMARY TABLE

CAS No. 1843-05-6	DATE	RESULTS	FULFILLS REQUIREMENT
PHYSICAL/CHEMICAL ELEMENTS			
Melting Point	2000	47 -49 °C	Yes
Boiling Point	1968	> 300 °C (Decomposes)	Not applicable
Vapour Pressure		--	Not applicable
Partition Coefficient	2000	Log Kow > 6.00	Yes
Water Solubility	2001	<7.3 x 10 ⁻⁷ g/L of solution at 20.0±0.5°C	Yes
ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS			
Photodegradation	2001	For reaction with hydroxyl radical, predicted rate constant = 218.14 x 10 ¹² cm ³ /molecule-sec predicted half-life = 0.59 h [EPIWIN Program]	Yes
Stability in Water	2001	The estimated half-life at pH 4, 7, and 9 at 25°C is > 1 year.	Yes
Fugacity	2000	Predicted distribution using Level III Fugacity model Air 0.09% Water 8.2% Soil 29.5% Sediment 62.2% [EPIWIN Program]	Yes
Biodegradation	1989	Not Biodegradable	Yes
ECOTOXICITY ELEMENTS			
Acute Toxicity to Fish	1988	Zebra fish (<i>Brachydanio rerio</i>): LC ₅₀ (96 h) > 100 mg/L	Yes
Toxicity to Aquatic Plants	1992	Green Algae (<i>Scenedesmus subspicatus</i>) EC ₅₀ (0 -72 h) > 100 mg/L	Yes
Acute Toxicity to Aquatic Invertebrates	1988	Daphnia magna Straus 1820 EC ₀ (24 h) > 10 mg/L EC ₅₀ (24 h) > 52 mg/L	Yes
MAMMALIAN TOXICITY			
Acute Toxicity	1965	>10 g/kg (rats)	Yes
Genetic Toxicity: Gene Mutations	1991	Non-mutagenic to bacterial cells	Yes
Genetic Toxicity: Chromosomal Aberration	2001	Non-clastogenic to human lymphocytes <i>in vitro</i>	Yes
Repeated Dose Toxicity	1965	Rat 30-day Dietary	Yes
	1965	Rat 90-day Dietary NOEL = 0.6 % (6000 ppm)	Yes
	1965	Dog 120-day Dietary NOEL = 0.6% (6000 ppm)	Yes
	1968	Rat 90-day Dietary NOEL = 0.15 % (1500 ppm)	Yes
	1969	Rats 90-day Dietary NOEL = 1000 ppm	Yes
Reproductive/ Developmental Toxicity	1969	Rats NOEL = 0.6% (6000 ppm) for 4 Successive Generations	Yes

PROPOSED TEST PLAN

CAS# 1843-05-6	Data Available	Data Acceptable	Testing Required
Study	Y/N	Y/N	Y/N
Physical/Chemical Characteristics			
Melting Point	Y	Y	N
Boiling Point	NA	NA	N
Vapor Pressure	NA	NA	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
Environmental Fate			
Photodegradation	Y	Y	N
Hydrolysis	Y	Y	N
Fugacity	Y	Y	N
Biodegradation	Y	Y	N
Ecotoxicity			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Invertebrates	Y	Y	N
Acute Toxicity to Algae	Y	Y	N
Mammalian Toxicity			
Acute Toxicity	Y	Y	N
Repeat Dose Toxicity	Y	Y	N
Genetic Toxicity: Gene Mutations	Y	Y	N
Genetic Toxicity: Chromosomal Aberration	Y	Y	N
Developmental Toxicity	Y	Y	N
Reproductive Toxicity	Y	Y	N

GENERAL INFORMATION

A. INTRODUCTION

On November 22 and 29, 1999, respectively, Cytec Industries Inc. (Cytec) and Ciba Specialty Chemicals Corporation (Ciba) agreed to participate in the Environmental Protection Agency's (EPA) High Production Volume Chemical Challenge Program. By participating in this program, Cytec and Ciba agreed to assess the adequacy of existing data, design and submit test plans to fill data gaps where necessary and appropriate, provide test results, and prepare summaries of the data characterizing each chemical sponsored.

The sponsored chemical addressed in this test plan is 2-hydroxy-4-n-octoxybenzophenone, (CAS # 1843-05-6).

B. GENERAL SUBSTANCE INFORMATION

Chemical Name: 2-hydroxy-4-n-octoxybenzophenone

Description: The substance is a pale, cream-to-white powder with friable lumps.

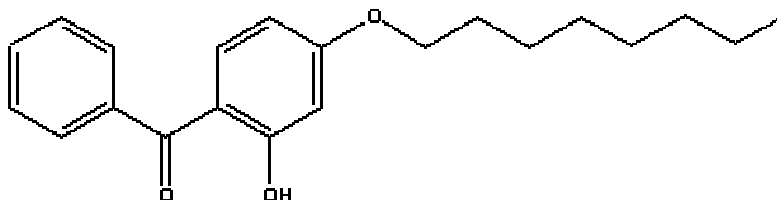
Chemical Abstract Service Registry Number: CAS # 1843-05-6

Common Name: Benzophenone-12

Chemical Formula: $C_{21}H_{26}O_3$

Molecular Weight: 326.42

Structure:



C. GENERAL USE INFORMATION

2-Hydroxy-4-n-octoxybenzophenone is an effective photostabilizer for a variety of plastic systems. It may be used in food packaging materials as an antioxidant and stabilizer and in addition may be used as a stabilizer in petroleum wax. As such, it is cleared under the 21 CFR (Code of Federal Regulations) §178.2010 for use as a stabilizer in polypropylene, polyethylene, olefin copolymers, and poly(methylpentene) complying with limitations set forth in §177.1520c and also under 21 CFR §178.3710. When used in packaging materials, 2-hydroxy-4-n-octoxybenzophenone prevents UV-radiation from reaching the stored product and increases the stability of the container. In order to be approved by the FDA for such uses, 2-hydroxy-4-n-octoxybenzophenone has been thoroughly evaluated for its potential toxicity.