

Environmental Assessment  
in Support  
of an Import Tolerance  
for Benzocaine in Food Derived from Atlantic  
Salmon and Rainbow Trout

ACD Pharmaceuticals, AS  
Storgata, 9  
8376 Leknes, Norway

May 11, 2017

## 1. General Information

Requestor: ACD Pharmaceuticals AS  
Storgata, 9  
8376 Leknes, Norway

Drug Established Name: Benzocaine

## 2. Purpose and Need for the Proposed Action

Benzocaine is the active pharmaceutical ingredient (API) in drugs such as BENZOAK<sup>1</sup>, which is approved for use as an anesthetic and sedative in salmon and rainbow trout in Norway. Aquaculture drugs containing benzocaine are also approved for use in Chile and Spain. The European Agency for the Evaluation of Medicinal Products (EMEA; now the European Medicines Agency, EMA), Committee for Veterinary Medicinal Products (CVMP), has concluded that there was no need to establish a maximum residue limit (MRL) for benzocaine when used as a local anesthetic and recommended it be included in Annex II of Council Regulation (EEC) No. 237/90 as a local anesthetic for all food-producing animals. In an October 3, 2000, submission to the EMEA, a request was made for the ruling to be extended to include use as a central (systemic) anesthetic in all fish of the family Salmonidae, which are collectively referred to as salmonids. This request was subsequently granted (EMEA, 2001) under the provision that the substance is not intended for use as an anesthetic and tranquilizer before slaughter for human consumption. Benzocaine is also acceptable for use via immersion in Canada for euthanasia of aquatic species that are not intended to be introduced into the food supply (Canadian Council on Animal Care).

Benzocaine is not currently approved or conditionally approved in the United States (US) as a drug substance for use in or on any fish species; therefore ACD Pharmaceuticals, S.A. is requesting establishment of an import tolerance for residues of benzocaine in Atlantic salmon and rainbow trout so that imported food derived from fish of these two species that have been treated with, and contain residues of, benzocaine may be legally marketed in the US for human consumption. The act of establishing an import tolerance is an agency action requiring the preparation of an environmental assessment (EA) unless the action is one that meets criteria for categorical exclusion under FDA regulations in 21 CFR Part 25, Subpart C, which is currently not the case. Therefore, the current EA has been prepared to address and evaluate potential direct and indirect environmental impacts in the US due to the action of establishing an import tolerance for residues of benzocaine in food derived from treated Atlantic salmon and rainbow trout.

The impact on the environment of the US arising from the occurrence of benzocaine residues in fish tissues will be evaluated herein based on the primary pathways for environmental exposure and the available physical-chemical property and fate data for the drug (Section 5). In addition, because use of benzocaine could potentially occur in countries adjacent to the US, Canada in particular, consideration will also be given to the potential for effects on the US environment as a result of benzocaine use in these other countries.

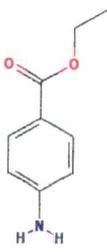
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<sup>1</sup> See Appendix 1 for specific information on BENZOAK.

### 3. Identification of the Substance

Benzocaine is an anesthetic that reversibly stabilizes the neuronal membrane which decreases its permeability to sodium ions. Depolarization of the neuronal membrane is inhibited thereby blocking the initiation and conduction of nerve impulses (NIH, 2016). Table 1 summarizes the most relevant physical-chemical properties of benzocaine.

Table 1. Select Chemical Characteristics of Benzocaine (NIH, 2016)

Chemical Name	ethyl p-aminobenzoate
Chemical Abstracts Service Number	94-09-7
Molecular formula	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
Molecular weight	165.19 g/mol
Chemical structure	
Water Solubility	1,310 mg/L at 25°C (Yalkowsky, 2003); 1,811 mg/L (EPI Suite, Appendix 2)
Log octanol-water partition coefficient (Log K <sub>ow</sub> )	1.86 (Hansch, 1995); 1.80 (EPI Suite, Appendix 2)
Organic-carbon normalized soil adsorption coefficient (K <sub>oc</sub> )	250 (estimated from log K <sub>ow</sub> of 1.86) (NLM, 2016)
Acid dissociation constant (pKa)	2.51 (Perrin, 1965)
Vapour pressure	2.6 x 10 <sup>-4</sup> mmHg at 25°C (EPI Suite, Appendix 2)

### 4. Sites of Introduction and Exposure Pathways

There are two general types of exposure pathways for benzocaine to the US environment that could potentially exist due to the establishment of an import tolerance for this drug in fish tissues: 1) pathways arising from the release of drug residues, if present, from imported food derived from treated fish, or 2) pathways arising from use of the drug on fish in countries where it is legally authorized. With respect to the first of the two general types of exposure pathways, i.e., following the importation of food derived from benzocaine-treated Atlantic salmon and rainbow trout, release of benzocaine into the US environment (e.g., soil, surface water, air) may potentially occur through two points of introduction:

- through landfills that may hold seized materials (fish or food-derived from treated fish) containing residues of the drug;

- through wastewater treatment plant effluents and biosolids that may contain residues of the drug from human excreta as a result of consumption of imported food from treated fish.

The potential introduction of drug residues into soils and surface waters from landfills and wastewater treatment facilities strongly depends on the inherent physicochemical and fate properties of the respective drug (e.g., water solubility, adsorption coefficients, biodegradation rates, etc.), as well as on numerous factors specific to the landfills (e.g., liner type and thickness, soil type, proximity to surface water) and wastewater treatment facilities themselves (e.g., removal efficiencies, flow rates, dilution factors). In general, only in cases where the drug is volatile or highly mobile (i.e., will migrate out of the compartments at the site of introduction), and present at concentrations high enough to cause effects, is it possible that environmental impacts on the circumjacent ecosystems could become evident.

The potential introduction of benzocaine to the US environment from the use of the drug on Atlantic salmon and rainbow trout in countries where it is legally authorized is unlikely to occur. Although benzocaine can be legally used in adjacent countries, specifically Canada, it is not expected to be used in food fish there because the drug has not been approved for use in food fish in Canada. In addition, the substantial dilution and spatial and temporal variability that would occur due to the distance the benzocaine would need to travel to reach US waters would likely eliminate any potential significant exposure to non-target organisms in the US.

The environmental exposure and likelihood of benzocaine to cause impacts on the ecosystems at the sites of introduction is evaluated in Section 5.

## **5. Analysis of Exposure and Risk**

The potential exposures due to the pathways listed in Section 4 will be evaluated based on the available metabolism and environmental fate data for benzocaine, which is described below. Information on the metabolism of benzocaine in fish will help to determine the types and magnitude of residues, if any, that could potentially be present in imported Atlantic salmon and rainbow trout tissues (which could be potentially be disposed of in landfills in the US), as well as the amount of the drug (and/or its potential metabolites) consumed by humans in the US, which could then be present in sewage and processed by wastewater treatment facilities, and subsequently be discharged to surface waters. The environmental fate information will help to determine if benzocaine is likely to migrate out of landfills, and whether it will likely be persistent in terrestrial and aquatic environments. In addition, fate information will also help determine the potential for exposure from the discharge of effluents and from applications of biosolids produced by wastewater treatment plants.

### **A. Metabolism and fate of benzocaine**

#### *Metabolism and residues in fish*

Several studies have been conducted examining the metabolism and residues in various fish species that have been treated with benzocaine (Hayton, 1996; Stehly, 2000; Allen, 1988). In Stehly, 2000, rainbow trout were treated first in a bath containing 30 mg/L benzocaine for 5 minutes, then in a bath containing 15 mg/L benzocaine for an additional 30 minutes. Elimination at two different temperatures, 7°C and 16°C, was

analyzed and there was no statistical difference in the results. Immediately after these treatments, the average fillet tissue residue was about 27 µg/g benzocaine. At 24 hours post-treatment, concentrations of benzocaine in the edible fillet tissue of all fish were below the limit of quantification of 22 ng/g. The concentration of the major metabolite, acetylated benzocaine, was also below the limit of quantification of 23 ng/g after 24 hours.

The rapid loss of benzocaine from trout fillet tissue is in agreement with previous studies in catfish (Hayton, 1996). In Hayton, 1996, catfish were exposed to 70 mg/L benzocaine until they lost the ability to hold themselves upright (normally about 5 minutes), and then to 35 mg/L benzocaine for an additional 30 minutes. The average concentration of benzocaine in the tissues and fluids immediately after exposure ranged from 19.4 ± 14.3 µg/g in white muscle to 143 ± 9.87 µg/g in liver. Most of the residue disappeared from the tissues and fluids rapidly, with concentrations declining to about 1% of their initial values by 25 hours after exposure, with the exception of bile, which had concentrations of residues around 387 ± 133 µg/g. It should be noted that benzocaine in bile is not of major concern because imported fish would most likely be gutted or processed prior to shipment and because filets are the typical fish product imported into the US.

Another study (Allen, 1988) measured the depletion of benzocaine (parent compound and metabolites) residues in muscle tissue of rainbow trout and largemouth bass. In Allen, 1988, fish were exposed to 50 mg benzocaine/L for 15 minutes in a static immersion water bath and then recovered in flowing, anesthetic-free water at 12°C. Residues of benzocaine peaked in both largemouth bass and rainbow trout at 1 hour post-dose and rapidly depleted to below mean control concentrations (0.47 ± 0.04 µg/g) of benzocaine in muscle tissue of largemouth bass at 8 hours post-dose, and were near mean control concentrations (0.44 ± 0.06 µg/g) in muscle tissue of rainbow trout at 4 hours post dose. According to the study, a background reading of benzocaine concentrations in the controls is caused by naturally occurring primary aromatic amines.

#### *Adsorption and mobility*

A  $K_{oc}$  of 250 L/kg was estimated based on the log  $K_{ow}$  of 1.86 and a regression-derived equation (Lyman, 1990). This  $K_{oc}$ , along with a water solubility of 1,310 mg/L and a log  $K_{ow}$  of 1.86, indicate that benzocaine is not expected to adsorb greatly to suspended solids and sediments in the aqueous environment. Likewise, for residues present in terrestrial environments, significant adsorption to soil is not expected and moderate mobility in soil is predicted.

#### *Degradation and persistence in water*

Benzocaine was classified as biodegradable in a procedure using an acclimated sludge inoculum, indicating that biodegradation may be an important fate process in the environment (Wotzka, 1993). Using the Estimation Program Interface (EPI) Suite, the hydrolysis half-life was estimated to be 9.156 years at pH 8 and 91.557 years at pH 7.<sup>2</sup> In addition, EPI Suite estimated that ultimate biodegradation<sup>3</sup> will occur within weeks and primary biodegradation<sup>4</sup> will occur within days to weeks. These EPI Suite estimates for biodegradation suggest that benzocaine will not be highly persistent in water.

<sup>2</sup> See Appendix 2 for EPI Suite results.

<sup>3</sup> Ultimate biodegradation is the transformation of a parent compound to carbon dioxide and water, mineral oxides of any other elements present in the test compound, and new cell material.

<sup>4</sup> Primary biodegradation is the transformation of a parent compound to an initial metabolite.

B. Exposure and risks for pathways arising from the release of benzocaine residues from imported food derived from treated Atlantic salmon and rainbow trout

As discussed previously, there are two theoretically possible pathways to the environment at large for benzocaine residues originating in imported food (e.g., fish steaks and filets):

- through release from landfills that may hold seized materials (fish or food-derived from treated fish) containing residues of the drug;
- through discharges via effluents or runoff from land application of biosolids from wastewater treatment that may contain residues of the drug in human excreta as a result of consumption of imported food from treated fish.

The amount of benzocaine introduced into the US environment from these pathways is expected to be extremely low because residues of benzocaine in muscle and skin of fish decline rapidly (e.g., within 24 hours) after treatment to very low levels. Therefore, the amount of residues in tissues at the time of slaughter and import into the US are expected to be *de minimus* and below detection limits.<sup>5</sup>

The potential for impacts to the US environment through these two exposure pathways is evaluated further below.

*Landfill*

Landfills in the US are highly regulated by local, state and federal authorities to prevent environmental contamination. For example, most landfills are required to have caps and liners of clay or an impermeable membrane to prevent leaching of water or fluids therein (and any contaminants they may contain) to groundwater and/or local surface waters (e.g., rivers and lakes). As a result of these controls and the fact that the amounts of residues in fish tissue will be extremely small, if not nonexistent, to begin with, there is expected to be minimal or no movement of benzocaine out of US landfills and into the adjacent US environment (groundwater or surface water). In addition, because benzocaine has a low vapor pressure ( $2.6 \times 10^{-4}$  mmHg at 25°C) and moderately high water solubility (1,310 mg/L), it is not expected to volatilize from landfills and enter air to any significant extent. Therefore, based on a lack of exposure, significant environmental impacts on the terrestrial and aquatic environments are not expected from residues of benzocaine in imported food derived from treated Atlantic salmon and rainbow trout that are disposed of in US landfills.

*Wastewater discharge and application of biosolids to land*

The concentrations of drug residues introduced into the US environment from effluents from wastewater treatment facilities, as well as application of biosolids obtained from wastewater treatment facilities, as a result of human consumption of imported food containing residues of benzocaine, is expected to be extremely low for several reasons. First, as previously described, the residues of benzocaine in muscle and tissue decline rapidly after treatment. Therefore, the amounts of residues in tissues at the time of import into the US are expected to be *de minimus* and below detection limits. Although the import tolerance itself is expected to be set at 50 ppb for residues in muscle, the

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<sup>5</sup> The European Medicines Agency has declined to establish a maximum residue limit (MRL) for benzocaine residues in fish tissues because residues are expected to be below the limit of detection even shortly after treatment.

actual tissue concentrations are likely to be much lower due to declines after treatment, which would typically occur days to weeks (or more) before fish are sacrificed and brought to market.

Additional reasons why this exposure pathway is not expected to be significant include: 1) further metabolism of benzocaine residues, if present, is likely to occur in humans after consumption; 2) the distribution of the excreted residues, if any, in the US environment will likely be spatially and temporally variable (i.e., it is very unlikely that enough Atlantic salmon and rainbow trout will be consumed in the same region on the same day to have a detectable level occurring in the same wastewater treatment facility); and 3) additional degradation and removal of benzocaine in wastewater treatment facilities. As a result, the expected concentrations of benzocaine entering the aquatic systems are expected to be extremely low, approaching zero (and likely undetectable), due to effluent as a result of discharge from wastewater treatment facilities and runoff from land applied biosolids. Further dilution of benzocaine is also expected to occur in effluent receiving waters. As a result, it is highly unlikely that benzocaine will ever be present at concentrations in water that would cause effects on aquatic life. Therefore, no significant environmental impacts to the aquatic environment are expected from this exposure pathway.

C. Exposure and risks to the US environment from use of benzocaine on Atlantic salmon and rainbow trout in countries where it is legally authorized

*Typical use conditions*

The typical use of benzocaine is as an anesthetic (sedative) in a static bath for vaccination and or examination purposes. Anesthesia in fish occurs by immersing fish in a static immersion bath at concentrations up to 40 mg benzocaine/L for up to 15 minutes. Usually there is only one application per fish at the time of vaccination; however, sedation may also be needed during other veterinary and health management procedures where handling is required. Disposal of benzocaine-treated water is mixed with effluent water from the hatchery and discharged according to permissions given to each hatchery from the proper authorities in that country.

*Analysis of potential impacts on the US environment*

As benzocaine has been approved for use in fish in seawater and freshwater in other countries, it has presumably undergone an evaluation as part of the approval processes in those countries to determine its potential impact on the aquatic environment.<sup>6</sup>

Once the fish have been treated and returned to their rearing tanks, the water in the static bath is mixed with hatchery effluent water, which greatly dilutes the concentration of benzocaine. The hatchery effluent is then discharged into a stream, ocean or bay further diluting the concentration of benzocaine. These discharges are regulated and/or permitted by the country of origin. In addition, while dilution occurs at various stages of the effluent discharge process and subsequent to discharge, it would also be expected that other physical and chemical processes (i.e. photolysis, hydrolysis, biodegradation, etc.) would occur concurrently to further limit the exposure of benzocaine to non-target organisms in the US environment. Because of this, impacts to the US environment from

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<sup>6</sup> The use of benzocaine in net pens in Canada (particularly in net pens on the Canada-US border) is not anticipated because use in food fish is not authorized in Canada, and because if used for vaccination this would be expected to occur in pre-smolts prior to their transfer from freshwater to seawater.

the use of benzocaine in foreign countries, including Canada which shares a boarder with the US, are highly unlikely.

## 6. Description of Any Alternatives to the Proposed Use

ACD Pharmaceuticals, S.D. is proposing to establish a tolerance for benzocaine in food derived from Atlantic salmon and rainbow trout that is imported into the US for human consumption. The only alternative to the proposed action is the 'no action' alternative, which would be the failure to establish a tolerance for benzocaine in Atlantic salmon and rainbow trout. However, based on our analysis in this EA, we do not believe that significant environmental impacts will occur from this action; therefore, the preferred alternative is the establishment of a tolerance for benzocaine in Atlantic salmon and rainbow trout imported into the US and the no action alternative was eliminated from consideration.

## 7. Conclusions

Based on the available information on the metabolism, environmental fate, and exposure of benzocaine, there is expected to be little or no exposure to benzocaine residues in the US environment for any of the exposure pathways evaluated. Therefore, it is concluded that the proposed action of establishing an import tolerance for benzocaine residues in Atlantic salmon and rainbow trout will not result in significant environmental impacts in the US.

## 8. Agencies and Persons Consulted

This EA was prepared with input and assistance from members of the Environmental Safety Team in the Office of New Animal Drug Evaluation in FDA's Center for Veterinary Medicine.

## 9. Preparer(s)

Mariann Dønnum  
George R. Kohan

## 10. Signature of Responsible Officials

The undersigned certifies that the information presented in this Environmental Assessment is to the best of their knowledge true, accurate and complete.

Signed Mariann Dønnum

Name: MARIANN DØNNUM

Title: CEO

Date: May 11th 2017

Signed GRK

Name: GEORGE R. KOHAN

Title: MANAGING DIRECTOR

Date: May 11, 2017



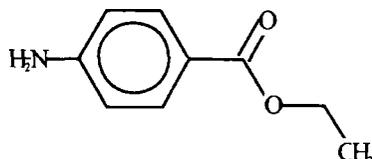
### **Appendix 1: BENZOAK (benzocaine) Drug Information**

The primary use of BENZOAK (benzocaine) in Norway is as an anesthetic in salmonid pre-smolts being given vaccines by injection. When vaccinated, these pre-smolts are between 35 to 100g in size and 12 to 24 months in age. BENZOAK is a stock solution (200 mg benzocaine/mL) that is diluted in a freshwater bath for immersion treatment of the fish. The dose will vary according to treatment conditions, such as water temperature, fish health, desirable induction time and fish size. The water temperature can vary between 1 to 18 °C and the anesthetic induction time decreases with an increase in water temperature. The approved dosage to induce sedation in approximately 2 to 5 minutes is 30 to 40 mg benzocaine/L (15 to 20 mL BENZOAK/100L). To induce sedation in approximately 45 to 60 seconds, a dose of up to 10 mL BENZOAK/10 liters of water can be used. After the fish have entered deep anesthesia, the fish will be flushed in clean freshwater to remove superficial surplus compound, injected (vaccinated) and transported to a tank for recovery. These fish are typically held in rearing tanks for 3 weeks to 5 months before they are transferred to marine net pens for grow-out.

Usually there is only one application per fish as pre-smolts; however, sedation may also be needed during other veterinary and health management procedures where handling is required. This use only affects small fractions of the fish population. For example, physical marking procedures (e.g. adipose fin clips) during the juvenile stage, or weight samples that may be carried out on several occasions during the rearing period. Another example is the use of BENZOAK or another anesthetic during routine salmon louse counts. These health management procedures typically involve sedation of 20 fish (out of 80,000-200,000 fish per marine net pen) every second week.

**Appendix 2: EPI Suite Results**

EPI Suite Results For CAS 000094-09-7



SMILES : O=C(OCC)c(ccc(N)c1)c1  
CHEM : Benzoic acid, 4-amino-, ethyl ester  
MOL FOR: C9 H11 N1 O2  
MOL WT : 165.19

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): -----  
Boiling Point (deg C) : -----  
Melting Point (deg C) : -----  
Vapor Pressure (mm Hg) : -----  
Water Solubility (mg/L): -----  
Henry LC (atm-m<sup>3</sup>/mole) : -----

Log Octanol-Water Partition Coef (SRC):  
Log Kow (KOWWIN v1.68 estimate) = 1.80  
Log Kow (Exper. database match) = 1.86  
Exper. Ref: HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 279.90 (Adapted Stein & Brown method)  
Melting Pt (deg C): 66.17 (Mean or Weighted MP)  
VP(mm Hg,25 deg C): 0.000258 (Modified Grain method)  
VP (Pa, 25 deg C) : 0.0345 (Modified Grain method)  
MP (exp database): 92 deg C  
BP (exp database): 310 deg C  
Subcooled liquid VP: 0.00115 mm Hg (25 deg C, Mod-Grain method)  
: 0.153 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 deg C (mg/L): 1671  
log Kow used: 1.86 (expkow database)  
no-melting pt equation used  
Water Sol (Exper. database match) = 1310 mg/L (30 deg C)

Exper. Ref: YALKOWSKY,SH & HE,Y (2003)

Water Sol Estimate from Fragments:  
Wat Sol (v1.01 est) = 1811.7 mg/L

ECOSAR Class Program (ECOSAR v1.11):  
Class(es) found:  
Anilines (Unhindered)  
Esters

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:  
Bond Method : 1.63E-008 atm-m<sup>3</sup>/mole (1.65E-003 Pa-m<sup>3</sup>/mole)  
Group Method: 9.96E-009 atm-m<sup>3</sup>/mole (1.01E-003 Pa-m<sup>3</sup>/mole)  
For Henry LC Comparison Purposes:  
User-Entered Henry LC: not entered  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 3.356E-008 atm-m<sup>3</sup>/mole (3.400E-003 Pa-m<sup>3</sup>/mole)  
VP: 0.000258 mm Hg (source: MPBPVP)  
WS: 1.67E+003 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:  
Log Kow used: 1.86 (exp database)  
Log Kaw used: -6.176 (HenryWin est)  
Log Koa (KOAWIN v1.10 estimate): 8.036  
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):  
Biowin1 (Linear Model) : 0.6093  
Biowin2 (Non-Linear Model) : 0.9446  
Expert Survey Biodegradation Results:  
Biowin3 (Ultimate Survey Model): 2.8394 (weeks )  
Biowin4 (Primary Survey Model) : 3.7300 (days-weeks )  
MITI Biodegradation Probability:  
Biowin5 (MITI Linear Model) : 0.4894  
Biowin6 (MITI Non-Linear Model): 0.4765  
Anaerobic Biodegradation Probability:  
Biowin7 (Anaerobic Linear Model): 0.2948  
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):  
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 0.153 Pa (0.00115 mm Hg)  
Log Koa (Koawin est ): 8.036  
Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):  
Mackay model : 1.96E-005  
Octanol/air (Koa) model: 2.67E-005  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model : 0.000706  
Mackay model : 0.00156  
Octanol/air (Koa) model: 0.00213

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 36.4601 E-12 cm<sup>3</sup>/molecule-sec

Half-Life = 0.293 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Half-Life = 3.520 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.00113 (Junge-Pankow, Mackay avg)

0.00213 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 58.98 L/kg (MCI method)

Log Koc: 1.771 (MCI method)

Koc : 73.57 L/kg (Kow method)

Log Koc: 1.867 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Total Kb for pH > 8 at 25 deg C : 2.399E-003 L/mol-sec

Kb Half-Life at pH 8: 9.156 years

Kb Half-Life at pH 7: 91.557 years

(Total Kb applies only to esters, carbmates, alkyl halides)

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 0.894 (BCF = 7.838 L/kg wet-wt)

Log Biotransformation Half-life (HL) = -1.5314 days (HL = 0.02941 days)

Log BCF Arnot-Gobas method (upper trophic) = 0.606 (BCF = 4.036)

Log BAF Arnot-Gobas method (upper trophic) = 0.606 (BAF = 4.036)

log Kow used: 1.86 (expkow database)

Volatilization from Water:

Henry LC: 9.96E-009 atm-m<sup>3</sup>/mole (estimated by Group SAR Method)

Half-Life from Model River: 7.555E+004 hours (3148 days)

Half-Life from Model Lake : 8.243E+005 hours (3.435E+004 days)

Removal In Wastewater Treatment:

Total removal: 2.14 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 2.04 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent) (hr) (kg/hr)

Air 0.148 7.04 1000

Water 23 360 1000

Soil 76.8 720 1000

Sediment 0.0977 3.24e+003 0

Persistence Time: 636 hr