



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
WASHINGTON, D.C. 20460

OFFICE OF  
PREVENTION, PESTICIDES AND  
TOXIC SUBSTANCES

March 18, 2005

**ACTION MEMORANDUM**

**SUBJECT:** Inert Ingredient Tolerance Reassessment – Glyceryl tris-12-hydroxystearate

**FROM:** Dan Rosenblatt, Chief  
Minor Use, Inerts, and Emergency Response Branch

**TO:** Lois A. Rossi, Director  
Registration Division

**I. FQPA REASSESSMENT ACTION**

**Action:** Reassessment of two (2) inert ingredient exemptions from the requirement of a tolerance.

**Chemical and Use Summary:** See table below.


Tolerance Exemptions Being Reassessed				
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use Pattern (Pesticidal)	List Classification
Glyceryl tris-12-hydroxystearate	139-44-6	180.920 <sup>1'</sup>	Flow control agent	4B
Glyceryl tris-12-hydroxystearate	139-44-6	180.930 <sup>2'</sup>	Flow control agent	4B

1. Residues listed in 40 CFR §180.920 [formerly 40 CFR§ 180.100(d)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops only.
2. Residues listed in 40 CFR §180.930 [formerly 40 CFR §180.1001(e)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations applied to animals.

**List Reclassification Determination:** Glyceryl tris-12-hydroxystearate is classified as a List 4B inert ingredient. Based on low overall toxicity concerns and the lack of absorption, and coupled with a lack of acute toxicity concerns for castor oil, an analogue of glyceryl tris-12-hydroxystearate, glyceryl tris-12-hydroxystearate can be reclassified as a List 4A inert ingredient.

## II. MANAGEMENT CONCURRENCE

I concur with the reassessment of the two (2) exemptions from the requirement of a tolerance for the inert ingredient, glyceryl tris-12-hydroxystearate, and with the List reclassification determination, as described above. I consider the two (2) exemptions from the requirement of a tolerance for glyceryl tris-12-hydroxystearate established in 40 CFR §180.920 [formerly 40 CFR§180.1001(d)] and in 40 CFR §180.930 [formerly 40 CFR§180.1001(e)] to be reassessed as of the date of my signature, below. A Federal Register Notice regarding this tolerance exemption reassessment decision will be published in the near future.



Lois A. Rossi, Director  
Registration Division

Date: 3.29.05

cc: Debbie Edwards, SRRD  
Joe Nevola, SRRD



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March 18, 2005

**MEMORANDUM**

SUBJECT: Reassessment of the Exemption from the Requirement of a Tolerance for  
Glyceryl tris-12-hydroxystearate

FROM: Kerry Leifer, Inerts Team Leader *[Signature]*  
Minor Use, Inerts and Emergency Response Branch  
Registration Division (7505C)

THRU: Pauline Wagner *Pauline Wagner 3/21/05*  
Registration Division (7505C)

TO: Dan Rosenblatt, Chief  
Minor Use, Inerts and Emergency Response Branch  
Registration Division (7505C)

**Background**

Attached is the science assessment for glyceryl tris-12-hydroxystearate. This assessment summarizes available information on the use, physical/chemical properties, toxicological effects, exposure profile, and environmental fate and ecotoxicity of glyceryl tris-12-hydroxystearate. The purpose of this document is to reassess the existing exemption from the requirement of a tolerance for residues of glyceryl tris-12-hydroxystearate as required under the Food Quality Protection Act (FQPA).

**Executive Summary**

This report evaluates glyceryl tris-12-hydroxystearate (CAS Reg. No.139-44-6), a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR

§180.920 [formerly 40 CFR §180.1001(d)] and 40 CFR §180.930 [formerly 40 CFR §180.1001(e)] for use as a flow control agent.

Glyceryl tris-12-hydroxystearate is a triester of glycerol and 12-hydroxystearic acid, a hydroxy fatty acid that is formed from the hydrogenation of the predominant castor oil fatty acid. Hydrogenation of castor oil results in a substance that is a waxy solid in nature which is also known as castor wax. In addition to its use as a pesticide product inert ingredient, glyceryl tris-12-hydroxystearate is used as a component of speciality wax blends like crayons, lipsticks, and stick deodorants.

A structure activity relationship (SAR) analysis of glyceryl tris-12-hydroxystearate was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that glyceryl tris-12-hydroxystearate was poorly absorbed via all routes of exposure and is of low concern for human health effects, with no identified health concerns. Glyceryl tris-12-hydroxystearate is water insoluble and readily degraded in the environment and would not be present in drinking water while also being of low concern for toxicity to aquatic organisms.

Taking into consideration all available information on glyceryl tris-12-hydroxystearate, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to glyceryl tris-12-hydroxystearate when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemptions from the requirement of a tolerance established for residues of glyceryl tris-12-hydroxystearate in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCFA.

## **I. Introduction**

This report evaluates glyceryl tris-12-hydroxystearate (CAS Reg. No. 139-44-6), a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR §180.920 [formerly 40 CFR §180.1001(d)] and 40 CFR §180.930 [formerly 40 CFR §180.1001(e)].

Glyceryl tris-12-hydroxystearate is a triester of glycerol and 12-hydroxystearic acid, a hydroxy fatty acid that is formed from the hydrogenation of the predominant castor oil fatty acid (O'Shea, 205). The chemical structure of glyceryl tris-12-hydroxystearate corresponds to fully hydrogenated castor oil. Hydrogenation of castor oil results in a substance that is a waxy solid in nature which is also known as castor wax. The hydrogenated form of castor oil has a wide array of uses including cosmetic and pharmaceutical applications.

## II. Use Information

### Pesticides

The tolerance exemptions for the inert ingredient glyceryl tris-12-hydroxystearate are given in Table 1 below.

<b>Table 1. Tolerance Exemption Being Reassessed in this Document</b>				
<b>Tolerance Exemption Expression</b>	<b>CAS Reg No.</b>	<b>40 CFR §</b>	<b>Use Pattern (Pesticidal)</b>	<b>List Classification</b>
Glyceryl tris-12-hydroxystearate	139-44-6	180.920 <sup>1/</sup>	Flow control agent	4B
Glyceryl tris-12-hydroxystearate	139-44-6	180.930 <sup>2/</sup>	Flow control agent	4B

1. Residues listed in 40 CFR §180.920 [formerly 40 CFR§ 180.100(d)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops only.
2. Residues listed in 40 CFR §180.930 [formerly 40 CFR §180.1001(e)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations applied to animals.

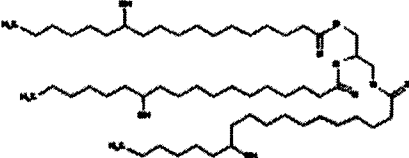
### Other Uses

Glyceryl tris-12-hydroxystearate is used as a component of speciality wax blends like crayons, lipsticks, and stick deodorants as well as being used in pharmaceuticals as an excipient in sustained release capsules. Other uses of glyceryl tris-12-hydroxystearate are as a thixotropic agent in paints, coatings, inks, adhesives, and sealants.

## III. Physical and Chemical Properties

Table 2 below lists some of the physical and chemical characteristics of glyceryl tris-12-hydroxystearate.

**Table 2. Physical and Chemical Properties of Glyceryl tris-12-hydroxystearate  
(CAS Reg. No 133-44-6)  
Measured (M) or Estimated (E)**

Parameter	Value	Source
Structure		ChemIDplus, 2005
Physical Form	Solid	OPPT, 2004
Molecular Weight	939.487	ChemIDplus, 2005
Water Solubility	$1.208 \times 10^{-17}$ mg/L at 25°C (E)	EPI Suite, 2004
Melting Point	349.84 °C (E)	EPI Suite, 2004
Henry's Law Constant	$5.6 \times 10^{-18}$ atm-m <sup>3</sup> /mole @25°C (E)	EP ISuite, 2004
Vapor Pressure	$1.14 \times 10^{-29}$ mmHg @25°C (E)	EPI Suite, 2004
Octanol/Water Partition Coefficient	log P = 19.73 (E)	EPI Suite, 2004

#### IV. Hazard Assessment

##### A. Hazard Profile

Glyceryl tris-12-hydroxystearate is a hydrogenated form of castor oil. There is no readily available toxicity data on glyceryl tris-12-hydroxystearate. Limited data are available on castor oil; as part of the Joint FAO/WHO Expert Committee on Food Additives (JECFA) evaluation of castor oil as a food additive, it was noted that while low doses of castor oil are absorbed by humans, higher doses are not absorbed and laxation is observed, consistent with its long history of use as a laxative (JECFA, 1979). A structure activity relationship analysis of glyceryl tris-12-hydroxystearate was conducted by the Office of Pollution Prevention and Toxics (OPPT) Structure Activity Team. The OPPT assessment concluded that glyceryl tris-12-hydroxystearate

was poorly absorbed via all routes of exposure and is of low concern for human health effects, with no identified health concerns (Appendix A).

## **B. Toxicological Data**

No references to toxicity studies on glyceryl tris-12-hydroxystearate were identified in the open literature.

## **C. Metabolism And Pharmacokinetics**

Glyceryl tris-12-hydroxystearate is expected to be poorly absorbed by the gastrointestinal (GI) tract (OPPT, 2004). While no pharmacokinetic data are available on glyceryl tris-12-hydroxystearate, as an orally-administered laxative, castor oil is not absorbed in the GI tract and is excreted unchanged in the feces. As part of its review of castor oil and derivatives as food additives, the European Commission's Scientific Committee for Food noted that small doses of castor oil are hydrolyzed and absorbed completely and can be stored and metabolized similar to dietary fatty acids (SCF, 2003).

## **D. Special Considerations for Infants and Children**

Glyceryl tris-12-hydroxystearate is poorly absorbed via all routes of exposure and is of low concern for human health effects, therefore a safety factor analysis has not been used to assess the risks resulting from the use of glyceryl tris-12-hydroxystearate and an additional tenfold safety factor for the protection of infants and children is unnecessary.

## **V. Exposure Assessment**

Glyceryl tris-12-hydroxystearate is poorly absorbed via all routes of exposure, therefore no further exposure assessment is necessary.

## **VI. Aggregate Exposures**

In examining aggregate exposure, FFDC section 408 directs EPA to consider available information concerning exposures from the pesticide residue in food and all other non-occupational exposures, including drinking water from ground water or surface water and exposure through pesticide use in gardens, lawns, or buildings (residential and other indoor uses).

For glyceryl tris-12-hydroxystearate, a qualitative assessment for all pathways of human exposure (food, drinking water, and residential) is appropriate given the lack of human health concerns associated with exposure to glyceryl tris-12-hydroxystearate.

## **VII. Cumulative Exposure**

Section 408(b)(2)(D)(v) of the FFDCFA requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to glyceryl tris-12-hydroxystearate and any other substances and this material does not appear to produce a toxic metabolite produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that glyceryl tris-12-hydroxystearate has a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at <http://www.epa.gov/pesticides/cumulative/>

#### **VIII. Environmental Fate Characterization/Drinking Water Considerations**

Glyceryl tris-12-hydroxystearate is water insoluble and undergoes ready biodegradation, and therefore would not be expected to be present in drinking water sources as a result of its use as a pesticide inert ingredient (EPI Suite, 2004). The estimated environmental fate properties of glyceryl tris-12-hydroxystearate are given in Appendix B.

#### **IX. Human Health Risk Characterization**

Glyceryl tris-12-hydroxystearate is a triglyceride that is similar to many other fats and oils and is the fully hydrogenated form of the predominant castor oil fatty acid. Glyceryl tris-12-hydroxystearate is not expected to be absorbed via any route of exposure and is of low concern for human health effects. Glyceryl tris-12-hydroxystearate is also readily degraded in the environment.

Taking into consideration all available information on glyceryl tris-12-hydroxystearate, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to glyceryl tris-12-hydroxystearate when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemptions from the requirement of a tolerance established for residues of glyceryl tris-12-hydroxystearate in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCFA.

#### **X. Ecotoxicity and Ecological Risk Characterization**



There are no available aquatic toxicity studies on glyceryl tris-12-hydroxystearate (ECOTOX, 2002); however, given the water insoluble nature of glyceryl tris-12-hydroxystearate, the OPPT Structure Activity Team rated glyceryl tris-12-hydroxystearate as low concern for toxicity to fish, algae, and aquatic invertebrates (Appendix A).

#### References:

ChemIDplus. 2005. ChemIDplus Advanced. U.S. National Library of Medicine. National Institutes of Health. Department of Health and Human Services. Online Search Database <http://chem.sis.nlm.nih.gov/chemidplus/>  
Search term: Glyceryl tris-12-hydroxystearate (February 13, 2005)

ECOTOX. 2002. U.S. Environmental Protection Agency. 2002. ECOTOX User Guide: ECOTOXicology Database System. Version 3.0. <http://www.epa.gov/ecotox/>  
Search terms: CAS Reg Nos: 139-44-6 (February 14, 2005)

EPI Suite. 2004. Estimation Programs Interface Suite Version 3.12 (August 17, 2004). Environmental Protection Agency. <http://www.epa.gov/opptintr/exposure/docs/episuite.htm>

JECFA. 1979. Joint FAO/WHO Expert Committee on Food Additives. Safety Evaluation of Certain Food Additives: Castor Oil. WHO Food Additive Series Vol. 14. World Health Organization, Geneva. <http://www.inchem.org/documents/jecfa/jecmono/v14je05.htm>

OPPT. 2004. Office of Pollution Prevention and Toxics Structure Activity Team Report: Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester. December 7, 2004

O'Shea. 2005. G. R. O'Shea Company. Castor Oil and its Chemistry. <http://www.groshea.com/caschemchemistry.html>

SCF. 2003. European Commission Scientific Committee on Food. Opinion of the Scientific Committee on Food on the 23rd Additional List of Monomers and Additives for Food Contact Material. Castor Oil and Some Derivatives. [http://europa.eu.int/comm/food/fs/sc/scf/out181\\_en.pdf](http://europa.eu.int/comm/food/fs/sc/scf/out181_en.pdf)

TOXNET 2005. Hazardous Substance Data Bank (HSDB). On-line Scientific Search Engine, National Library of Medicine, National Institute of Health. <http://www.toxnet.nlm.nih.gov>.  
Search term: Glyceryl tris-12-hydroxystearate

## STRUCTURE ACTIVITY TEAM REPORT

12/08/04

CASE NUMBER: Z05-0004

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	1	1

KEYWORDS:

SUMMARY OF ASSESSMENT

FATE: Solid  
 S (mg/L, 25°C) < 0.001(ICB); H < 1.00E-8(E)  
 BP (C) > 400(E); VP @ 25C (mm) < 1.0E-6(E)  
 POTW removal (%) = 50-75 via sorption and biodeg  
 Time for complete ultimate aerobic biodeg = wk  
 PBT Potential: P1B1T1  
 Sorption to soils/sediments = v.strong  
 \*CEB FATE: Migration to ground water = negl

HEALTH: Expect poor absorption via all routes. No significant health concerns.

\*CEB HEALTH: Low concern

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

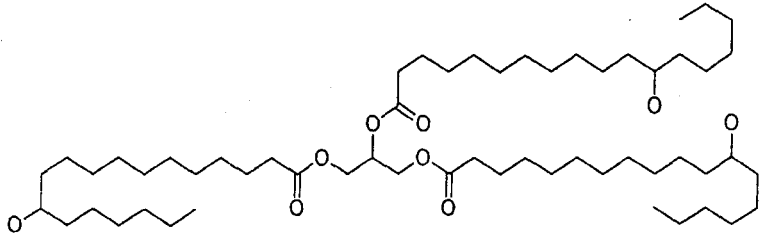
fish 96-h LC50	=	*	P
daphnid 48-h LC50	=	*	P
green algal 96-h EC50	=	*	P
fish chronic value	=	*	P
daphnid ChV	=	*	P
algal ChV	=	*	P

Predictions are based on SARs for esters; SAR chemical class = ester-tri-lipid-C17(OH); MW940; log Kow = 1.9 (ClogP); solid with mp unk (P); pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;  
 low concern for toxicity;  
 assessment factor = 10.0  
 concern concentration = \*  
 \*CEB ECOTOX: No releases to water

SAT Co-chair: Leonard Keifer 564-8916

## APPENDIX A

### OPPT SAT Review of Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester

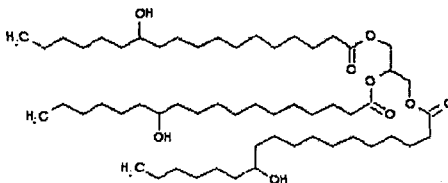
<b>STRUCTURE ACTIVITY TEAM REPORT</b>		ver. 04/98	<b>CBI? (YES/NO)</b>
<b>Case #:</b>	Z-05-0004	<b>DCN:</b>	
<b>SAT Date:</b>	12/7/2004	<b>SAT Chair:</b>	L. Keifer
<b>Submitter:</b>			
<b>Chemical Name:</b>			
Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester			
<b>CAS RN:</b>		<b>Trade Name:</b>	
139-44-6			
<b>Structure</b>			
			
<b>Molecular Formula:</b>		C <sub>57</sub> H <sub>110</sub> O <sub>9</sub>	
<b>Molecular Wt.</b>	940	<b>WT%&lt;500:</b>	<b>WT%&lt;1000:</b>
<b>MP:</b>		<b>BP:</b>	>500 <b>Eq. Wt:</b>
<b>H2O Sol (g/L):</b>	<0.000001	<b>V.P.</b>	<0.000001
<b>Max. Prod. Volume (kg/yr):</b>		<b>Physical State:</b>	Solid
<b>USE:</b>			
Pesticide Inert.			
<b>Related Case Numbers</b>	<b>Case Role</b>	<b>Related Case Numbers</b>	<b>Case Role</b>
<b>FOCUS</b>	<b>Date:</b>	<b>Results:</b>	

Page of

NCSAB SAT REPORT		CBI? (Y/N):	
PMN: Z-05-0004	CAS RN:		139-44-6
Chemical Name: Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester		Analog:	
		Production Volume:	
Structure:			
Use:			
Pesticide Inert.			
Formula: C <sub>57</sub> H <sub>110</sub> O <sub>9</sub>	Eq Wt:		
Mol Weight: 939.51	Wt% < 500:	Wt% < 1000	
MP:	BP:	> 500	VP: < 0.000001
H <sub>2</sub> O Sol (g/L): < 0.000001	Physical State:		Solid Log P: 19 (CLOGP)
Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	*		
Daphnid 48-h	*		
Algal 96-h	*		
Fish ChV	*		
Daphnid ChV	*		
Algal ChV	*		
BCF			
CHEMICAL CLASS:		SAR: ester - hydroxy - lipid	
ECOTOX CONCERN	H	M	(L) CONCERN CONCENTRATION *
DATE 12/7/04	ASSESSOR:		


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Full Record**

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[TOXNET](#)
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**Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester**  
**RN: 139-44-6**

**Names and Synonyms**
**Synonyms**

- 12-Hydroxyoctadecanoic acid, glyceryl ester
- 12-Hydroxyoctadecanoic acid, triester with glycerol
- 12-Hydroxystearic acid triglyceride
- AI3-19740
- EINECS 205-364-6
- Glycerol tris(12-hydroxystearate)
- Glyceryl tris(12-hydroxystearate)
- NSC 2389
- Octadecanoic acid, 12-hydroxy-, triester with glycerol
- Thixcin E
- Thixin R

**Systematic Name**

- 1,2,3-Propanetriyl tris(12-hydroxyoctadecanoate)
- Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester

**Superlist Name**

- Glyceryl tris(12-hydroxystearate)

**Registry Numbers**
**CAS Registry Number**
 139-44-6

**Other Registry Number**
 38264-86-7

**System Generated Number**
 000139446

**Formulas**
**Molecular Formula**
 C57-H110-O9

**Locators**
**File Locator**

## APPENDIX B

### Estimated Environmental Fate Properties of Glyceryl tris-12-hydroxystearic acid

SMILES : CCCCCC(CCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCC(O)CCCCC)OC(=O)CCCCCCCC  
CCC(O)CCCCC)O

CHEM : Octadecanoic acid, 12-hydroxy-, 1,2,3-propanetriyl ester

CAS NUM: 000139-44-6

MOL FOR: C57 H110 O9

MOL WT : 939.51

----- EPI SUMMARY (v3.12) -----

#### Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m<sup>3</sup>/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

#### Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = 19.73

#### Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C): 916.64 (Adapted Stein & Brown method)

Melting Pt (deg C): 349.84 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 1.14E-029 (Modified Grain method)

#### Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1.208e-017

log Kow used: 19.73 (estimated)

no-melting pt equation used

#### Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 9.3951e-007 mg/L

#### ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:

Esters

#### Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 6.90E-011 atm-m<sup>3</sup>/mole

Group Method: 5.60E-018 atm-m<sup>3</sup>/mole

Henrys LC [VP/WSol estimate using EPI values]: 1.023E+002 atm-m<sup>3</sup>/mole

#### Probability of Rapid Biodegradation (BIOWIN v4.02):

Biowin1 (Linear Model) : 1.6243

Biowin2 (Non-Linear Model) : 1.0000

#### Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.9185 (weeks )

Biowin4 (Primary Survey Model) : 4.3747 (hours-days )

Readily Biodegradable Probability (MITI Model):

Biowin5 (MITI Linear Model) : 1.5528  
Biowin6 (MITI Non-Linear Model): 0.9963

Ready Biodegradability Prediction: YES

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 99.7356 E-12 cm<sup>3</sup>/molecule-sec

Half-Life = 0.107 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Half-Life = 1.287 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 1E+010

Log Koc: 12.093

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Total Kb for pH > 8 at 25 deg C : 1.455E-001 L/mol-sec

Kb Half-Life at pH 8: 55.135 days

Kb Half-Life at pH 7: 1.510 years

BCF Estimate from Log Kow (BCFWIN v2.15):

Log BCF = 0.500 (BCF = 3.162)

log Kow used: 19.73 (estimated)

Volatilization from Water:

Henry LC: 6.9E-011 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)

Half-Life from Model River: 2.601E+007 hours (1.084E+006 days)

Half-Life from Model Lake : 2.837E+008 hours (1.182E+007 days)

Removal In Wastewater Treatment:

Total removal: 94.04 percent

Total biodegradation: 0.78 percent

Total sludge adsorption: 93.26 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0843	2.57	1000
Water	3.67	360	1000
Soil	29.5	720	1000
Sediment	66.8	3.24e+003	0

Persistence Time: 1.28e+003 hr