

The Green Chemical Company
111 Dash St.
Anywhere, VA 00000

Document Control Officer
Mail Stop 7407 – OPPT
TSCA Data Processing Center
Room 6428 EPA East
U.S. Environmental Protection Agency
1201 Constitution Ave., N.W.
Washington, DC 20004-3302

March 30, 2005

This PMN is being submitted under the Sustainable Futures Initiative

Dear Madam or Sir,

Enclosed is a Pre-Manufacture Notification (PMN) filed by The Green Chemical Company. No claims of confidentiality are being made on any of the enclosed information. This PMN is being submitted under the Sustainable Futures Initiative, and includes the Sustainable Futures Summary Assessment Worksheet and the results from all SF models used to evaluate this chemical. Information on how the Sustainable Futures chemical risk screening model results helped our company develop this notification, and the benefits realized by our company by using these screening models, is described on the Pollution Prevention page of this notification, and in the paragraph below.

The chemical that is the subject of this notification was the only candidate chemical available to our company that met performance, cost, and availability requirements. By using the ECOSAR model to estimate potential aquatic hazard, and ChemSTEER and E-FAST to estimate surface water releases and potential aquatic risk, we determined that, as an acrylate, this chemical presents potential aquatic toxicity concerns. In order to control potential aquatic risk, our company will process this chemical in a way that will restrict surface water releases to 1 day per year as a result of annual cleaning of the reactor vessel.

Attachments to this notification are listed below. If you have any questions, please contact George Bird at (555) 888-5555.

Sincerely,

Beverly R. Cardinal

Beverly R. Cardinal
Manager, Product Processing

Attachments:

Sustainable Futures Summary Assessment Worksheet
Print outs of SF Model runs: EPI Suite; PBT Profiler; ECOSAR; OncoLogic; ChemSTEER; E-FAST

<p>U.S. ENVIRONMENTAL PROTECTION AGENCY</p> <p>PREMANUFACTURE NOTICE</p> <p>FOR NEW CHEMICAL SUBSTANCES</p> <p>When completed send this form to</p> <p>DOCUMENT CONTROL OFFICER OFFICE OF POLLUTION PREVENTION AND TOXIC SUBSTANCES, 7407 U.S. E.P.A. 1200 Pennsylvania, NW WASHINGTON, D.C. 20460</p>	<p>AGENCY USE ONLY</p> <p>Date of receipt</p>
<p>Enter the total number of pages in the Premanufacture Notice</p> <p style="text-align: center; font-size: 24px; font-weight: bold;">▶ 18</p>	<p>Document control number</p> <p>EPA case number</p>

GENERAL INSTRUCTIONS

TS - 8 A C 3 1 T

- You must provide all information requested in this form to the extent that it is known to or reasonably ascertainable by you. Make reasonable estimates if you do not have actual data.
- Before you complete this form, you should read the "Instructions Manual for Premanufacture Notification" (the Instructions Manual is available from the Toxic Substances Control Act (TSCA) Information Service by calling 202-554-1404, or faxing 202-554-5603).
- If a user fee has been remitted for this notice (40 CFR 700.45), indicate in the boxes above the TS-user fee identification number you have generated. Remember, your user fee ID number must also appear on your corresponding fee remittance, which is sent to EPA, Washington Financial Management Center (3303), P.O. 360399M, Pittsburgh, PA 15251-6399, Attn. TSCA User fee.

Part I — GENERAL INFORMATION

You must provide the currently correct Chemical Abstracts (CA) Name of the new chemical substance, even if you claim the identity as confidential. You may authorize another person to submit chemical identity information for you, but your submission will not be complete and the review will not begin until EPA receives this information. A letter in support of your submission should reference your TS user fee identification number. You must submit an original and two copies of this notice including all test data. If you claimed any information as confidential, a single sanitized copy must also be submitted.

Part II — HUMAN EXPOSURE AND ENVIRONMENTAL RELEASE

If there are several manufacture, processing, or use operations to be described in Part II, sections A and B of this notice, reproduce the sections as needed.

Part III — LIST OF ATTACHMENTS

Attach additional sheets if there is not enough space to answer a question fully. Label each continuation sheet with the corresponding section heading. In Part III, list these attachments, any test data or other data and any optional information included in the notice.

OPTIONAL INFORMATION

You may include any information that you want EPA to consider in evaluating the new substance. On page 11 of this form, space has been provided for you to describe pollution prevention and recycling information you may have regarding the new substance.

So-called "binding" boxes are included throughout this form for you to indicate your willingness to be bound to certain statements you make in this section, such as use, production volume, protective equipment . . . This option is intended to reduce delays that routinely accompany the development of consent orders or Significant New Use Rules. Except in the case of exemption applications (such as TMEA, LVE, LOREX) where certain information provided in such notification is binding on the submitter when the Agency approves the exemption application, checking a binding box in this notice does not by itself prohibit the submitter from later deviating from the information (except chemical identity) reported in the form.

CONFIDENTIALITY CLAIMS

You may claim any information in this notice as confidential. To assert a claim on the form, mark (X) the confidential box next to the information that you claim as confidential. To assert a claim in an attachment, circle or bracket the information you claim as confidential. If you claim information in the notices as confidential, you must also provide a sanitized version of the notice, (including attachments) For additional instructions on claiming information as confidential, read the Instructions Manual

Mark (X) if any information in this notice is claimed as confidential

TEST DATA AND OTHER DATA

You are required to submit all test data in your possession or control and to provide a description of all other data known to or reasonably ascertainable by you, if these data are related to the health and environmental effects on the manufacture, processing, distribution in commerce, use, or disposal of the new chemical substance. Standard literature citations may be submitted for data in the open scientific literature. Complete test data (written in English), not summaries of data, must be submitted if they do not appear in the open literature. You should clearly identify whether test data is on the substance or on an analog. Also, the chemical composition of the tested material should be characterized. Following are examples of test data and other data. Data should be submitted according to the requirements of §720.50 of the Premanufacture Notification Rule (40 CFR Part 720).

Test Data (Check Below any included in this notice)

- Environmental fate data Yes
 - Other data Yes
 - Health effects data Yes
 - Risk assessments
 - Environmental effects data Yes
 - Structure/activity relationships
 - Physical/Chemical Properties* Yes
 - Test data not in the possession or control of the submitter
- * A physical and chemical properties worksheet is located on the last page of this form.

TYPE OF NOTICE (Check Only One)

- PMN (Premanufacture Notice)
- INTERMEDIATE PMN (submitted in sequence with final product PMN)
- SNUN (Significant New Use Notice)
- TMEA (Test Marketing Exemption Application)
- LVE (Low Volume Exemption) @ 40 CFR 723.50(c)(1)
- LOREX (Low Release/Low Exposure Exemption) @ 40 CFR 723.50(c)(2)
- LVE Modification LOREX Modification

IS THIS A CONSOLIDATED PMN? Yes

of chemicals or polymers 1
(Prenotice Communication # required, enter # on page 3)

Public reporting burden for this collection of information is estimated to average 110 hours per response, including time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding the burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Director, Collection Strategies Division (2822), U.S. Environmental Protection Agency, 1200 Pennsylvania Ave., N.W., Washington, D.C. 20460; and to the Office of Management and Budget, Paperwork Reduction Act (2070-0012), Washington, D.C. 20503.

CERTIFICATION -- A Printed copy of this signature page, with original signature, must be submitted

I certify that to the best of my knowledge and belief:

1. The company named in Part I, section A, subsection 1a of this notice form intends to manufacture or import for a commercial purpose, other than in small quantities solely for research and development, the substance identified in Part I, Section B.
2. All information provided in this notice is complete and truthful as of the date of submission.
3. I am submitting with this notice all test data in my possession or control and a description of all other data known to or reasonably ascertainable by me as required by §720.50 of the Premanufacture Notification Rule.

Additional Certification Statements:

If you are submitting a PMN, Intermediate PMN, Consolidated PMN, or SNUN, check the following **user fee** certification statement that applies:

- The Company named in Part I, Section A has remitted the fee of \$2500 specified in 40 CFR 700.45(b), or
- The Company named in Part I, Section A has remitted the fee of \$1000 for an Intermediate PMN (defined @ 40 CFR 700.43) in accordance with 40 CFR 700.45(b), or
- The Company named in Part I Section A is a small business concern under 40 CFR 700.43 and has remitted a fee of \$100 in accordance with 40 CFR 700.45(b).

If you are submitting a **low volume exemption (LVE)** application in accordance with 40 CFR 723.50(c)(1) or a **Low release and low exposure exemption (LoRex)** application in accordance with 40 CFR 723.50(c)(2), check the following certification statements:

- The manufacturer submitting this notice intends to manufacture or import the new chemical substance for commercial purposes, other than in small quantities solely for research and development, under the terms of 40 CFR 723.50.
- The manufacturer is familiar with the terms of this section and will comply with those terms; and
- The new chemical substance for which the notice is submitted meets all applicable exemption conditions.
- If this application is for an LVE in accordance with 40 CFR 723.50(c)(1), the manufacturer intends to commence manufacture of the exempted substance for commercial purposes within 1 year of the date of the expiration of the 30 day review period.

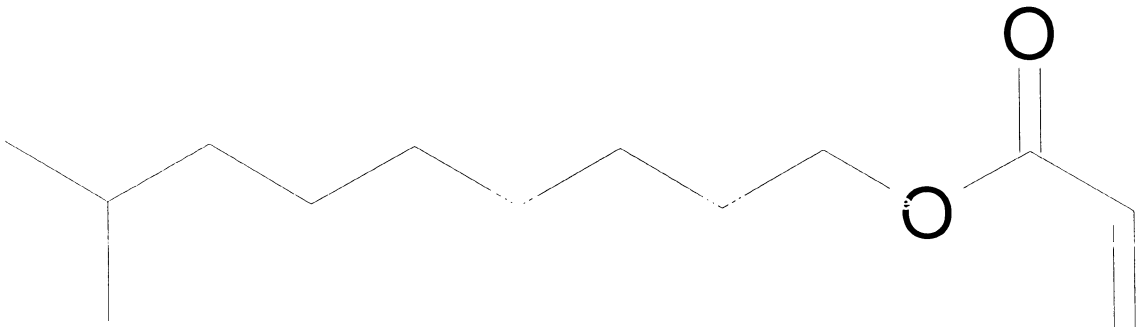
The accuracy of the statements you make in this notice should reflect your best prediction of the anticipated facts regarding the chemical substance described herein. Any knowing and willful misinterpretation is subject to criminal penalty pursuant to 18 USC 1001.

		Confidential
Signature and title of Authorized Official (Original Signature Required)	Date	<input type="checkbox"/>
Signature of agent - (if applicable)	Date	<input type="checkbox"/>

Part I -- GENERAL INFORMATION

Section A -- SUBMITTER IDENTIFICATION			Confidential
Mark () the "Confidential" box next to any subsection you claim as confidential			<input type="checkbox"/>
ia. Person Submitting Notice (in U.S.)	Name of authorized official Beverly R. Cardinal	Position Manager, Product Processing	<input type="checkbox"/>
	Company The Green Chemical Company		
	Mailing address (number and street) 111 Dash St.		
	City, State Anywhere, VA	Postal Code 00000	
b. Agent (if applicable)	Name of authorized official	Position	<input type="checkbox"/>
	Company		
	Mailing address (number and street)		
	City, State	Postal Code	Telephone (include area code)
c. If you are submitting this notice as part of a joint submission, mark (X) this box. → <input type="checkbox"/>			
Joint Submitter (if applicable)	Name of authorized official	Position	<input type="checkbox"/>
	Company		
	Mailing address (number and street)		City, State
	Province, Country	Postal Code	Telephone (include country or area code)
	2. Technical Contact (in U.S.)		
Name of authorized official George Bird		Position	
Company			
Mailing address (number and street)			
City, State		Postal Code	Telephone (include area code) 555-888-5555
3. If you have had a prenotice communication (PC) concerning this notice and EPA assigned a PC Number to the notice, enter the number. →		Mark (X) if none →	<input type="checkbox"/>
4. If you previously submitted an exemption application for the chemical substance covered by this notice, enter the exemption number assigned by EPA. If you previously submitted a PMN for this substance enter the PMN number assigned by EPA (i.e. withdrawn or incomplete). →		Mark (X) if none →	<input type="checkbox"/>
5. If you have submitted a notice of Bona fide intent to manufacture or import for the chemical substance covered by this notice, enter the notice number assigned by EPA. →		Mark (X) if none →	<input type="checkbox"/>
6. Type of Notice - Mark (X)		1. <input type="checkbox"/> Manufacture Only <input type="checkbox"/> Binding Option Mark (X)	2. <input checked="" type="checkbox"/> Import Only <input type="checkbox"/> Binding Option Mark (X)
		3. <input type="checkbox"/> Both	

Part I -- GENERAL INFORMATION -- Continued

Section B -- CHEMICAL IDENTITY INFORMATION:		You must provide a currently correct Chemical Abstracts (CA) name of the substance based on the ninth Collective Index (9CI) of CA nomenclature rules and conventions	
Mark (X) the "Confidential" box next to any item you claim as confidential			
Complete either item 1 (Class 1 or 2 substances) or 2 (Polymers) as appropriate. Complete all other items.			
If another person will submit chemical identity information for you (for either Item 1 or 2), mark (X) the box at the right. Identify the name, company, and address of that person in a continuation sheet.			<input type="checkbox"/>
			Confidential
1. Class 1 or 2 chemical substances (for definitions of class 1 and class 2 substances, see the Instructions Manual)			
a. Class of substance - Mark (X)		<input checked="" type="checkbox"/>	Class 1 or <input type="checkbox"/>
		<input type="checkbox"/>	Class 2
b. Chemical name (Currently correct Chemical Abstracts (CA) Name that is consistent with TSCA Inventory listings for similar substances. For Class 1 substances a CA Index Name must be provided. For Class 2 substances either a CA Index Name or CA Preferred Name must be provided, which ever is appropriate based on CA 9CI nomenclature rules and conventions).			<input type="checkbox"/>
2-Propenoic acid, isodecyl ester			
c. Please identify which method you used to develop or obtain the specified chemical identity information reported in this notice: (check one).			
<input type="checkbox"/> Method 1 (CAS Inventory Expert Service - a copy of the Identification report obtained from the CAS Inventory Expert Services must be submitted as an attachment to this notice)		<input checked="" type="checkbox"/>	Method 2 (Other Source)
d. Molecular formula		CBI	CAS Registry Number (if a number already exists for the substance)
C13H24O2		<input type="checkbox"/>	1330-61-6
e. For a class 1 substance, provide a complete and correct chemical structure diagram. For a class 2 substance, provide a correct representative or partial chemical structure diagram, as complete as can be known, if one can be reasonably ascertained. Please see the E-PMN Instruction Manual for discussion of "native format" diagram software which can be helpful in reviewing your substance.			<input type="checkbox"/>
			
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet			

PMN Page 4a ; Page 5 of 18

For a class 2 substance - (1) List the immediate precursor substances with their respective CAS Registry Numbers. (2) Describe the nature of the reaction or process. (3) Indicate the range of composition and the typical composition (where appropriate).

e. (1) List the immediate precursor substances with their respective CAS Registry Numbers.
Name (CAS #)

Confidential

e. (2) Describe the nature of the reaction or process.

e. (3) Indicate the range of composition and the typical composition (where appropriate).

Mark (X) this box if you attach a continuation sheet

Part I -- GENERAL INFORMATION -- Continued

Section B -- CHEMICAL IDENTITY INFORMATION -- Continued

2. Polymers (For a definition of polymer, see the Instructions Manual.)

a. Indicate the number-average weight of the lowest molecular weight composition of the polymer you intend to manufacture. Indicate maximum weight percent of low molecular weight species (not including residual monomers, reactants, or solvents) below 500 and below 1,000 absolute molecular weight of that composition.

Describe the methods of measurement or the basis for your estimates: GPC Other : (Specify below)

(i) lowest number average molecular weight: _____

(ii) maximum weight % below 500 molecular weight: _____

(iii) maximum weight % below 1000 molecular weight: _____

Confidential

Mark (X) this box if you attach a continuation sheet.

b. You must make separate confidentiality claims for monomer or other reactant identity, composition information, and residual information. Mark (X) the "Confidential" box next to any item you claim as confidential

- (1) - Provide the specific chemical name and CAS Registry Number (if a number exists) of each monomer or other reactant used in the manufacture of the polymer.
- (2) - Mark (X) this column if entry in column (1) is confidential.
- (3) - Indicate the typical weight percent of each monomer or other reactant in the polymer.
- (4) - Choose "yes" from drop down menu if you want a monomer or other reactant used at two weight percent or less to be listed as part of the polymer description on the TSCA Chemical Substance Inventory.
- (5) - Mark (X) this column if entries in columns (3) and (4) are confidential.
- (6) - Indicate the maximum weight percent of each monomer or other reactant that may be present as a residual in the polymer as manufactured for commercial purposes.
- (7) - Mark (X) this column if entry in column (6) is confidential.

Monomer or other reactant and CAS Registry Number (1)	Confidential (2)	Typical composition (3)	Include in identity (4)	Confidential (5)	Maximum residual (6)	Confidential (7)
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>
	<input type="checkbox"/>	%	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>

Mark (X) this box if you attach a continuation sheet

<p>c. Please identify which method you used to develop or obtain the specified chemical identity information reported in this notice (check one). <input type="checkbox"/> Method 1 (CAS Inventory Expert Service - a copy of the identification report obtained from CAS Inventory Expert Service must be submitted as an attachment to this notice) <input type="checkbox"/> Method 2 (other source)</p>	<p>CBI <input type="checkbox"/></p>
<p>d. The currently correct Chemical Abstracts (CA) name for the polymer that is consistent with TSCA Inventory listings for similar polymers.</p>	<p><input type="checkbox"/></p>
<p>CAS Registry Number (if a number already exists for the substance)</p>	<p><input type="checkbox"/></p>
<p>e. Provide a correct representative or partial chemical structure diagram, as complete as can be known, if one can be reasonably ascertained. Please see the E-PMN Instruction Manual for discussion of "native format" diagram software which can be helpful in reviewing your substance.</p>	<p><input type="checkbox"/></p>
<div style="border: 1px solid black; height: 500px; width: 100%;"></div>	
<p><input type="checkbox"/> Mark (X) this box if you attach a continuation sheet.</p>	

Part I -- GENERAL INFORMATION -- Continued

Section B -- CHEMICAL IDENTITY INFORMATION -- Continued

3. Impurities

- (a) - Identify each impurity that may be reasonably anticipated to be present in the chemical substance as manufactured for commercial purpose. Provide the CAS Registry Number if available. If there are unidentified impurities, enter "unidentified."
- (b) - Estimate the maximum weight % of each impurity. If there are unidentified impurities, estimate their total weight %

Impurity and CAS Registry Number (a)	Maximum percent (b)	Confidential
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>
	%	<input type="checkbox"/>

Mark (X) this box if you attach a continuation sheet.

4. Synonyms - Enter any chemical synonyms for the new chemical identified in subsection 1 or 2.

Isodecyl alcohol, acrylate; Acrylic acid, isodecyl ester;
Isodecyl propenoate; Isodecyl acrylate

Confidential

Mark (X) this box if you attach a continuation sheet.

5. Trade identification - List trade names for the new chemical substance identified in subsection 1 or 2.

MyCure 3310

Mark (X) this box if you attach a continuation sheet.

6. Generic chemical name - If you claim chemical identity as confidential, you must provide a generic name for your substance that reveals the specific chemical identity of the new chemical substance to the maximum extent possible. Refer to the TSCA Chemical Substance Inventory, 1985 Edition, Appendix B for guidance on developing generic names.

Mark (X) this box if you attach a continuation sheet.

7. Byproducts - Describe any byproducts resulting from the manufacture, processing, use, or disposal of the new chemical substance. Provide the CAS Registry Number if available.

Byproduct (1)	CAS Registry Number (2)	Confidential
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>

Mark (X) this box if you attach a continuation sheet.

Part I -- GENERAL INFORMATION -- Continued

Section C -- PRODUCTION, IMPORT, AND USE INFORMATION:

Mark (X) the "Confidential" box next to any item you claim as confidential.

1. Production volume -- Estimate the **maximum** production volume during the first 12 months of production. Also estimate the maximum production volume for any consecutive 12-month period during the first three years of production. Estimates should be on 100% new chemical substance basis. For a Low Volume Exemption application, if you choose to have your notice reviewed at a lower production volume than 10,000 kg/yr, specify the volume and mark (x) in the binding box. If granted, you are bound to this volume

Maximum first 12-month production (kg/yr) (100% new chemical substance basis)	Maximum 12-month production (kg/yr) (100% new chemical substance basis)	Confidential	Binding Option Mark (x)
11,200	11,200	<input type="checkbox"/>	<input type="checkbox"/>

2. Use Information -- You must make separate confidentiality claims for the description of the category of use, the percent of production volume devoted to each category, the formulation of the new substance, and other use information. Mark (X) the "Confidential" Box next to any item you claim as confidential.
 a. (1) --Describe each intended category of use of the new chemical substance by function and application. (2) --Mark (X) this column if entry column (1) is confidential business information (CBI). (3) --Indicate your willingness to have the information provided in column (1) binding. (4) --Estimate the percent of total production for the first three years devoted to each category of use. (5) --Mark (X) this column if entry in column (4) is confidential business information (CBI). (6) --Estimate the percent of the new substance as formulated in mixtures, suspensions, emulsions, solutions, or gels as manufactured for commercial purposes at sites under your control associated with each category of use. (7) --Mark (X) this column if entry in column (6) is confidential business information (CBI). (8) --Indicate % of product volume expected for the listed "use" sectors. Mark more than one box if appropriate. Mark (X) to indicate your willingness to have the use type provided in (8) binding. (9) --Mark (X) this column if entry(ies) in column (8) is (are) confidential business information (CBI).

Category of use (1) (by function and application i.e. a dispersive dye for finishing polyester fibers)	CBI (2)	Binding Option Mark (x) (3)	Production % (4)	CBI (5)	% in Formulation (6)	CBI (7)	% of substance expected per use (8)					CBI (9)	
							Site-limited	Consumer	Industrial	Commercial	Binding Option		
Reactive diluent in radiation curable coatings, adhesives, etc.	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	30	<input type="checkbox"/>			100			<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	%	<input type="checkbox"/>						<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	%	<input type="checkbox"/>						<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	%	<input type="checkbox"/>						<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	%	<input type="checkbox"/>						<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>	<input type="checkbox"/>	%	<input type="checkbox"/>	%	<input type="checkbox"/>						<input type="checkbox"/>	<input type="checkbox"/>

* If you have identified a "consumer" use, please provide on a continuation sheet a detailed description of the use(s) of this chemical substance in consumer products. In addition include estimates of the concentration of the new chemical substance as expected in consumer products and describe the chemical reactions by which this substance loses its identity in the consumer product

Mark (X) this box if you attach a continuation sheet

b. Generic use description If you claim any category of use description in subsection 2a as confidential, enter a generic description of that category. Read the Instruction Manual for examples of generic use descriptions.

Mark (X) this box if you attach a continuation sheet

3. Hazard Information -- Include in the notice a copy of reasonable facsimile of any hazard warning statement, label, material safety data sheet, or other information which will be provided to any person who is reasonably likely to be exposed to this substance regarding protective equipment or practices for the safe handling, transport, use, or disposal of the new substance. List in part III hazard information you include.

Mark (X) this box if you attach hazard information

Binding Option Mark (x)

Part II-- HUMAN EXPOSURE AND ENVIRONMENTAL RELEASE

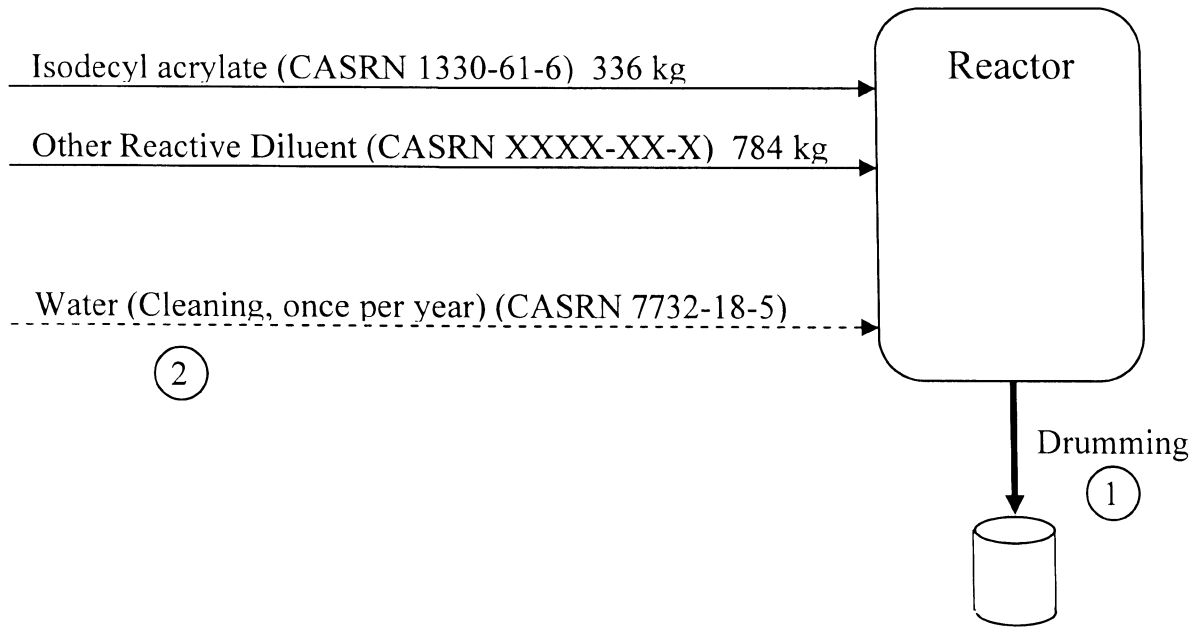
Section A -- INDUSTRIAL SITES CONTROLLED BY THE SUBMITTER

Mark (X) the "Confidential" box next to any item you claim as confidential

Complete section A for each type of manufacture, processing, or use operation involving the new chemical substance at industrial sites you control. Importers do not have to complete this section for operations outside the U.S.; however, you may still have reporting requirements if there are further industrial processing or use operations after import. You must describe these operations. See instructions manual

1. Operation description			Confidential
a. Identity -- Enter the identity of the site at which the operation will occur.			
Name			<input type="checkbox"/>
Site address (number and street)			
City, County, State, ZIP code			
If the same operation will occur at more than one site, enter the number of sites. Identify the additional sites on a continuation sheet, and if any of the sites have significantly different production rates or operations, include all the information requested in this section for those sites as attachments. →			<input type="checkbox"/>
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet.			
b. Type --			<input type="checkbox"/>
Mark (X) <input type="checkbox"/> Manufacturing <input checked="" type="checkbox"/> Processing <input type="checkbox"/> Use			<input type="checkbox"/>
c. Amount and Duration -- Complete 1 or 2 as appropriate			
1. Batch	Maximum kg/batch (100% new chemical substance) 1120	Hours/batch 24	Batches/year 10
2. Continuous	Maximum kg/day (100% new chemical substance)	Hours/day	Days/year
d. Process description <input type="checkbox"/> Mark (X) to indicate your willingness to have your process description binding.			<input type="checkbox"/>
(1) Diagram the major unit operation steps and chemical conversions. Include interim storage and transport containers (specify- e.g. 5 gallon pails, 55 gallon drum, rail car, tank truck, etc.). (2) Provide the identity, the approximate weight (by kg/day or kg/batch on a 100% new chemical substance basis), and entry point of all starting materials and feedstocks (including reactants, solvents, catalysts, etc.), and of all products, recycle streams, and wastes. Include cleaning chemicals (note frequency if not used daily or per batch). (3) Identify by number the points of release, including small or intermittent releases, to the environment of the new chemical substance. If releasing to two media at the same step, assign a second release number for the second medium.			
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet			

Confidential



Part II-- HUMAN EXPOSURE AND ENVIRONMENTAL RELEASE -- Continued

Section A -- INDUSTRIAL SITES CONTROLLED BY THE SUBMITTER -- Continued

2. **Occupational Exposure** -- You must make separate confidentiality claims for the description of worker activity, physical form of the new chemical substance, number of workers exposed, and duration of activity. Mark (X) the "Confidential" box next to any item you claim as confidential.
 (1) -- Describe the activities (i.e. bag dumping, tote filling, unloading drums, sampling, cleaning, etc.) in which workers may be exposed to the substance.
 (2) -- Mark (X) this column if entry in column (1) is confidential business information (CBI).
 (3) -- Describe any protective equipment and engineering controls used to protect workers.
 (4) and (6) -- Indicate your willingness to have the information provided in column (3) or (5) binding.
 (5) -- Indicate the physical form(s) of the new chemical substance (e.g., solid: crystal, granule, powder, or dust) and % new chemical substance (if part of a mixture) at the time of exposure.
 (7) -- Mark (X) this column if entry in column (5) is confidential business information (CBI).
 (8) -- Estimate the maximum number of workers involved in each activity for all sites combined.
 (9) -- Mark (X) this column if entry in column (8) is confidential business information (CBI).
 (10) and (11) -- Estimate the maximum duration of the activity for any worker in hours per day and days per year.
 (12) -- Mark (X) this column if entries in columns (10) and (11) are confidential business information (CBI).

Worker activity (i.e., bag dumping, filling drums) (1)	CBI (2)	Protective Equipment/ Engineering Controls (3)	Binding Option Mark (x) (4)	Physical forms(s) and % new substance (5)	Binding Option Mark (x) (6)	CBI (7)	# of Workers Exposed (8)	CBI (9)	Maximum	duration	CBI (12)
									Hrs/day (10)	Days/yr (11)	
Charging Reactor		Fugitive Emissions Recovery Equipment		Liquid 100%			1			10	
Filling Drums				Soluti on 30%			1			10	
Cleaning Reactor				Soluti on 30%			1			1	

Mark (X) this box if you attach a continuation sheet

3. Environmental Release and Disposal -- You must make separate confidentiality claims for the release number and the amount of the new chemical substance released and other release and disposal information. Mark (X) the "Confidential" box next to each item you claim as confidential.

(1) -- Enter the number of each release point identified in the process description, part II, section A, subsection 1d(3).

(2) -- Estimate the amount of the new substance released (a) directly to the environment or (b) into control technology (in kg/day or kg/batch).

(3) -- Mark (X) this column if entries in columns (1) and (2) are confidential business information (CBI).

(4) -- Identify the media (stack air, fugitive air (optional-see Instruction Manual), surface water, on-site or off-site land or incineration, POTW, or other (specify)) to which the new substance will be released from that release point.

(5) -- a. Describe control technology, if any, and control efficiency that will be used to limit the release of the new substance to the environment. For releases disposed of on land, characterize the disposal method and state whether it is approved for disposal of RCRA hazardous waste. On a continuation sheet, for each site describe any additional disposal methods that will be used and whether the waste is subject to secondary or tertiary on-site treatment. b. Estimate the amount released to the environment after control technology (in kg/day).

(6) -- Mark (X) this column if entries in columns (4) and (5) are confidential business information (CBI).

(7) -- Identify the destination(s) of releases to water. Please supply NPDES (National Pollutant Discharge Elimination System) numbers for direct discharges or NPDES numbers of the POTW (Publicly Owned Treatment Works). Mark (X) if the POTW name or NPDES # is confidential business information (CBI).

Release Number (1)	Amount of new substance released		CBI (3)	Medium of release e.g. stack air (4)	Control technology and efficiency (you may wish to optionally attach efficiency data)			CBI (6)
	(2a)	(2b)			(5a)	Binding Mark (X)	(5b)	
1	9.7E-4 kg/d		<input type="checkbox"/>	Fugitive Air		<input type="checkbox"/>		<input type="checkbox"/>
2	3.3E-3 kg/d		<input type="checkbox"/>	Fugitive Air		<input type="checkbox"/>		<input type="checkbox"/>
2	11 kg/d		<input type="checkbox"/>	Surface Water		<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>			<input type="checkbox"/>		<input type="checkbox"/>

(7) Mark (X) the destination(s) of releases to water.		NPDES #	CBI
<input checked="" type="checkbox"/> POTW--provide name(s)	Archway City Water Treatment Facility	XY0047029	<input type="checkbox"/>
<input type="checkbox"/> Navigable waterway--provide name(s)			<input type="checkbox"/>
<input type="checkbox"/> Other--Specify			<input type="checkbox"/>
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet			

Part II-- HUMAN EXPOSURE AND ENVIRONMENTAL RELEASE -- Continued

Section B -- INDUSTRIAL SITES CONTROLLED BY OTHERS

Complete section B for typical processing or use operations involving the new chemical substance at sites you do not control. Importers do not have to complete this section for operations outside the U.S.; however, you must report any processing or use activities after import. See the Instructions Manual. *Complete a separate section B for each type of processing, or use operation involving the new chemical substance.* If the same operation is performed at more than one site describe the typical operation common to these sites. Identify additional sites on a continuation sheet.

1(a). Operation Description -- To claim information in this section as confidential, circle or bracket the specific information that you claim as confidential.
 (1) -- Diagram the major unit operation steps and chemical conversions, including interim storage and transport containers (specify - e.g. 5 gallon pails, 55 gallon drums, rail cars, tank trucks, etc). On the diagram, identify by letter and briefly describe each worker activity. (2) -- Either in the diagram or in the text field 1(b) below, provide the identity, the approximate weight (by kg/day or kg/batch, on an 100% new chemical substance basis), and entry point of all feedstocks (including reactants, solvents and catalysts, etc) and all products, recycle streams, and wastes. Include cleaning chemicals (note frequency if not used daily or per batch). (3) -- Either in the diagram or in the text field 1(b) below, identify by number the points of release, including small or intermittent releases, to the environment of the new chemical substance. (4) Please enter the # of sites (remember to identify the locations of these sites on a continuation sheet):

_____ / # of sites

CBI

Diagram the major unit operation steps and chemical conversions...

1(b) (Optional) This space is for a text description to clarify the diagram above.

Mark (X) this box if you attach a continuation sheet

2. Worker Exposure/Environmental Release
 (1) -- From the diagram above, provide the letter for each worker activity. Complete 2-8 for each worker activity described.
 (2) -- Estimate the number of workers exposed for all sites combined.
 (4) -- Estimate the typical duration of exposure per worker in (a) hours per day and (b) days per year
 (6) -- Describe physical form of exposure and % new chemical substance (if in mixture), and any protective equipment and engineering controls, if any, used to protect workers.
 (7) -- Estimate the percent of the new substance as formulated when packaged or used as a final product.
 (9) -- From the process diagram above, enter the number of each release point. Complete 9-13 for each release point identified.
 (10) -- Estimate the amount of the new substance released (a) directly to the environment or (b) into control technology to the environment (in kg/day or kg/batch)
 (12) -- Describe media of release i.e. stack air, fugitive air (optional-see Instructions Manual), surface water, on-site or off-site land or incineration, POTW, or other (specify) and control technology, if any, that will be used to limit the release of the new substance to the environment.
 (14) -- Identify byproducts which may result from the operation.
 (3), (5), (8), (11), (13) and (15) -- Mark (X) this column if any of the preceding entries are confidential business information (CBI).

Letter of Activity (1)	# of Workers Exposed (2)	CBI (3)	Duration Of Exposure		CBI (5)	Protective Equip. /Engineering Controls/Physical Form and/ % new substance (6)	% in Formulation (7)	CBI (8)
			(4a)	(4b)				
		<input type="checkbox"/>			<input type="checkbox"/>			<input type="checkbox"/>
		<input type="checkbox"/>			<input type="checkbox"/>			<input type="checkbox"/>
		<input type="checkbox"/>			<input type="checkbox"/>			<input type="checkbox"/>
		<input type="checkbox"/>			<input type="checkbox"/>			<input type="checkbox"/>
		<input type="checkbox"/>			<input type="checkbox"/>			<input type="checkbox"/>

Release Number (9)	Amount of New Substance Released		CBI (11)	Media of Release & Control Technology (12)	CBI (13)
	(10a)	(10b)			
			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>		<input type="checkbox"/>
			<input type="checkbox"/>		<input type="checkbox"/>

(14) -- Byproducts:
 (15)

Mark (X) this box if you attach a continuation sheet.

OPTIONAL POLLUTION PREVENTION INFORMATION

To claim information in the following section as confidential circle or bracket the specific information that you claim as confidential.

In this section you may provide information not reported elsewhere in this form regarding your efforts to reduce or minimize potential risks associated with activities surrounding manufacturing, processing, use and disposal of the PMN substance. Please include new information pertinent to pollution prevention, including source reduction, recycling activities and safer processes or products available due to the new chemical substance. Source reduction includes the reduction in the amount or toxicity of chemical wastes by technological modification, process and procedure modification, product reformulation, raw materials substitution, and/or inventory control. Recycling refers to the reclamation of useful chemical components from wastes that would otherwise be treated or released as air emissions or water discharges, or land disposal. Descriptions of pollution prevention, source reduction and recycling should emphasize potential risk reduction subsequent to compliance with existing regulatory requirements and can be either quantitative or qualitative. The EPA is interested in the information to assess overall net reductions in toxicity or environmental releases and exposures, not the shifting of risks to other environmental media or non-environmental areas (e.g., occupational or consumer exposure). In addition, information on the relative cost or performance characteristics of the PMN substance to potential alternatives may be provided.

All information provided in this section will be taken into consideration during the review of this substance. See PMN Instructions Manual and Pollution Prevention Guidance manual for guidance and examples.

Optional Pollution Prevention Information (Continued) Describe the expected net benefits, such as (1) an overall reduction in risk to human health or the environment; (2) a reduction in the volume manufactured; (3) a reduction in the generation of waste materials through recycling, source reduction or other means; (4) a reduction in potential toxicity or human exposure and/or environmental release; (5) an increase in product performance, a decrease in the cost of production and/or improved operation efficiency of the new chemical substance in comparison to existing chemical substances used in similar application; or (6) the extent to which the new chemical substance may be a substitute for an existing substance that poses a greater overall risk to human health or the environment.

CBI

Mark (X) this box if you attach a continuation sheet.

Part III -- LIST OF ATTACHMENTS

Attach continuation sheets for sections of the form and test data and other data (including physical/chemical properties and structure/activity information), and optional information after this page. Clearly identify the attachment and the section of the form to which it relates, if appropriate. Number consecutively the pages of any paper attachments. In the column below, enter the inclusive page numbers of each attachment. Electronic attachments can be identified by filename.
 Mark (X) the "Confidential" box next to any attachment name you claim as confidential. Read the Instructions Manual for guidance on how to claim any information in an attachment as confidential. You must include with the sanitized copy of the notice form a sanitized version of any attachment in which you claim information as confidential.

#	Attachment name	Attachment Filename	Attachment page number(s)	Confidential
1	Physical and Chemical Properties Worksheet		13	<input type="checkbox"/>
2	Sustainable Futures Summary Assessment		14-27	<input type="checkbox"/>
				<input type="checkbox"/>
	[Attachments 3-8: P2 Framework Model outputs]			<input type="checkbox"/>
3	EPIWIN (EPISuite) Physicochem Prop/Environmental Fate		28-30	<input type="checkbox"/>
4	PBT Profiler: Environmental Fate/Distribution		31-32	<input type="checkbox"/>
5	ECOSAR: Aquatic Toxicity QSAR		33-34	<input type="checkbox"/>
6	OncoLogic: Carcinogenicity Potential SAR		35-37	<input type="checkbox"/>
7	ChemSTEER: Occupational Exposure & Environ Release		38-40	<input type="checkbox"/>
8	E-FAST: Aquatic & General Population Exposure		41-47	<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
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				<input type="checkbox"/>
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet Enter the attachment name and number				

PHYSICAL AND CHEMICAL PROPERTIES WORKSHEET

To assist EPA's review of physical and chemical properties data, please complete the following worksheet for data you provide and include it in the notice. Identify the property measured, the page of the notice on which the property appears, the value of the property, the units in which the property is measured (as necessary), and whether or not the property is claimed as confidential. If the attachments are electronic, give the attachment number (found on page 12) at (b). The physical state of the neat substance should be provided. These measured properties should be for the neat (100% pure) chemical substance. Properties that are measured for mixtures or formulations should be so noted (% PMN substance in). You are not required to submit this worksheet; however, EPA strongly recommends that you do so, as it will simplify review and ensure that confidential information is properly protected. You should submit this worksheet as a supplement to your submission of test data. This worksheet is not a substitute for submission of test data.

Property (a)	Mark (X) if provided	Page number (b)	Value (c)	Measured or Estimate (M or E)	Confidential Mark (X) (d)
Physical state of neat substance	<input checked="" type="checkbox"/>		<input type="checkbox"/> (s) <input checked="" type="checkbox"/> (l) <input type="checkbox"/> (g)		<input type="checkbox"/>
Vapor pressure @ Temperature ²⁵ °C	<input checked="" type="checkbox"/>		0.0227 Torr	E	<input type="checkbox"/>
Density/relative density	<input type="checkbox"/>		g/cm3		<input type="checkbox"/>
Solubility @ Temperature _____ °C Solvent _____	<input type="checkbox"/>		g/L		<input type="checkbox"/>
Solubility in water @ Temperature ²⁵ °C	<input checked="" type="checkbox"/>		0.00303 g/L	E	<input type="checkbox"/>
Melting temperature	<input checked="" type="checkbox"/>		-100 °C	M	<input type="checkbox"/>
Boiling / sublimation temperature @ ⁵⁰ torr pressure	<input checked="" type="checkbox"/>		158 °C	M	<input type="checkbox"/>
Spectra	<input type="checkbox"/>				<input type="checkbox"/>
Dissociation constant	<input type="checkbox"/>				<input type="checkbox"/>
Particle size distribution	<input type="checkbox"/>				<input type="checkbox"/>
Octanol / water partition coefficient	<input checked="" type="checkbox"/>		5.07	E	<input type="checkbox"/>
Henry's Law constant	<input checked="" type="checkbox"/>		1.2E-03 atm-m3/mol	E	<input type="checkbox"/>
Volatilization from water	<input type="checkbox"/>				<input type="checkbox"/>
Volatilization from soil	<input type="checkbox"/>				<input type="checkbox"/>
pH @ concentration _____	<input type="checkbox"/>				<input type="checkbox"/>
Flammability	<input type="checkbox"/>				<input type="checkbox"/>
Explosibility	<input type="checkbox"/>				<input type="checkbox"/>
Adsorption / coefficient	<input type="checkbox"/>				<input type="checkbox"/>
Other - Specify	<input type="checkbox"/>				<input type="checkbox"/>
Other - Specify	<input type="checkbox"/>				<input type="checkbox"/>
<input type="checkbox"/> Mark (X) this box if you attach a continuation sheet. Enter the attachment name and number.					

Attachment 2

Sustainable Futures Summary Assessment

Sustainable Futures

Summary Assessment

Using

P2 Framework Models

This document was developed to help compile estimation results from U.S. EPA OPPT's P2 Framework Models www.epa.gov/oppt/p2framework/ and is used by OPPT during Sustainable Futures (SF) training described at www.epa.gov/opptintr/newchems/sustainablefutures.htm. Participants in the voluntary SF Pilot Project are asked to submit the information contained in this assessment along with their SF PMNs in their choice of format.

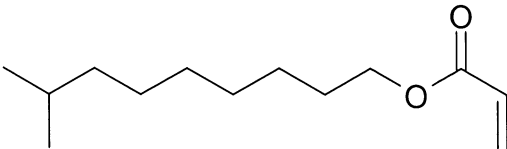
Use of this specific format is not mandatory.

Chemical Assessed:
2-Propenoic Acid, Isodecyl Ester

CAS Registry Number:
1330-61-6

Participant Name:
The Green Chemical Company

Date of Assessment:
03/25/2005

Record ID: GCC001		CAS No. 1330-61-6	
<p style="text-align: center;">Chemical Structure</p>  <p style="text-align: center;">Is this a representative structure? No</p>		MW: 212.34	
		MF: C ₁₃ H ₂₄ O ₂	
		Physical Form: Liquid	
		Submitter: The Green Chemical Company	
		Trade Name: MyCure 3310	
		Use: Reactive diluent in radiation curable coatings, adhesives, etc.	
		Production Volume: 11,200	
SMILES: CC(C)CCCCCCCOC(=O)C=C			
Name: 2-Propenoic acid, isodecyl ester			
Synonyms: (1) Isodecyl alcohol, acrylate (2) Acrylic acid, isodecyl ester (3) Isodecyl propenoate (4) Isodecyl acrylate			
SUSTAINABLE FUTURES SUMMARY:			
Concern Level	HIGH	MODERATE	LOW
Persistence			X
Bioconcentration			X
Cancer Health Hazard			X
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard	X		
Is the chemical predicted to be a PBT by PBT Profiler?	No		
Overall Hazard Concern	Human Health Hazard: Moderate Aquatic Hazard: High		
Overall Risk	Human Health Risk: Low Aquatic Risk: Low		

CAS No. 1330-61-6	Submitter: The Green Chemical Company
PHYSICAL/CHEMICAL PROPERTIES:	
Melting Point (deg C)	-100 (experimental)
Boiling Point (deg C)	158 (experimental)
Boiling Point Pressure (mm Hg)	50 (experimental)
Vapor Pressure (mm Hg)	2.27×10^{-2} (EPI)
Water Solubility (g/L)	0.00303 (EPI)
Log K_{ow}	5.07 (EPI)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC ($\text{atm}\cdot\text{m}^3/\text{mol}$)	1.2×10^{-3} (EPI)
Soil Adsorption Coefficient – log K_{oc}	3.1 (EPI)
Bioconcentration Factor – BCF	161.1 (EPI)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Weeks (EPI)
Primary Biodeg Model	Days (EPI)
Atmospheric Half-life	17 hours [rxn with OH radicals] (EPI)
Hydrolysis Half-life	>1 year (EPI)
Volatilization Half-life for Model River	2.2 hours (EPI)
Volatilization Half-life for Model Lake	6 days (EPI)
Removal in Sewage Treatment Plant	99.9% (EPI)
Ready Biodegradability	Ready Biodegradable (EPI)
Byproducts	
Degradation Products	Acrylic acid; isodecyl alcohol
Metabolites	

CAS No. 1330-61-6	Submitter: The Green Chemical Company
ECOTOXICITY:	
ECOSAR Class	Acrylates
Acute Toxicity	
Fish LC ₅₀	0.90 mg/L, 96-hr (ECOSAR)
Daphnid LC ₅₀	0.55 mg/L, 48-hr (ECOSAR)
Green Algae EC ₅₀	0.07 mg/L, 96-hr (ECOSAR)
Chronic Toxicity	
Fish ChV	0.005 mg/L, 32-day (ECOSAR)
Daphnid ChV	0.06 mg/L, 48-hr LC ₅₀ /10 (ECOSAR)
Green Algae ChV	0.02 mg/L, 96-hr EC ₅₀ /4 (ECOSAR)
Overall Hazard Concern for Aquatic Toxicity	High
CANCER HEALTH EFFECTS:	
Experimental data	Low by analogy to isooctyl acrylate (Gordon et al 1991)
OncoLogic Results	Marginal
Overall Hazard Concern for Carcinogenicity	Low
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low by analogy to isooctyl acrylate, based on acute LD ₅₀ >5000 mg/kg for rats by oral gavage (IUCLID 29590-42-9)
Irritation	Positive by analogy to isooctyl acrylate (Gordon et al. 1991)
Skin Sensitizer	Positive based on dermal sensitization of analogs in lab animals and humans (8e-11424, 8e-14572, 8e-3774)
Reproductive Effects	No relevant data identified
Developmental Effects	Moderate by analogy to isooctyl acrylate, which produced skeletal variations in the offspring of rats treated orally during pregnancy; LOAEL = 1,000 mg/kg-day (8e-1524)
Immune System Effects	No relevant data identified
Neurotoxicity	No relevant data identified
Genotoxicity	Negative by analogy to isooctyl acrylate and hexyl acrylate (CCRIS)
Mutagenicity	No relevant data identified
Systemic Effects	No relevant data identified
Overall Hazard Concern for Non-Cancer Health Effects	Moderate

CAS No. 1330-61-6		Submitter: The Green Chemical Company	
EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	User-defined Processing	Number of Release Days	10
SIC Code / NPDES #		Number of Facilities	1
Occupational Exposure Values			
	Cancer LADD	Chronic ADD	Acute APDR
Dermal	0.118 mg/kg-day	0.207 mg/kg-day	7.56 mg/kg-day
Inhalation	3.12×10^{-3} mg/kg-day	5.45×10^{-3} mg/kg-day	0.199 mg/kg-day
Environmental Release Values			
Release to Water	11 kg/year (11 kg/site-day over 1 day/yr)		
Release to Air (Fugitive) [drumming]	0.0097 kg/year (9.7×10^{-4} kg/site-day over 10 days/yr)		
Release to Air (Fugitive) [reactor cleaning]	0.0033 kg/year (3.3×10^{-3} kg/site-day over 1 day/yr)		
Release to Landfill			
Release from Incineration			
Other Release Activities			
GENERAL POPULATION EXPOSURE VALUES: E-FAST			
Aquatic Exposure:			
Lowest Acute COC – Aquatic Exposure	20 µg/L (green algae acute/4, rounded to 1 sig. digit)		
Lowest Chronic COC – Aquatic Exposure	1 µg/L (fish chronic value/10, rounded to 1 sig. digit)		
Predicted Environmental Concentration (PEC)	2.82 µg/L		
PEC Exceeds Chronic COC (days / year)	<1		
Human Exposure:			
	Cancer LADDpot	Chronic ADDpot	Acute ADRpot
Drinking Water	1.89×10^{-8} mg/kg-day	4.73×10^{-8} mg/kg-day	1.50×10^{-4} mg/kg-day
Fish Ingestion	1.31×10^{-8} mg/kg-day	3.27×10^{-8} mg/kg-day	2.56×10^{-4} mg/kg-day
Fugitive Emissions [drumming]	9.77×10^{-11} mg/kg-day	2.44×10^{-10} mg/kg-day	
Fugitive Emissions [reactor cleaning]	3.36×10^{-12} mg/kg-day	8.41×10^{-12} mg/kg-day	
Incineration Emissions			
Landfill Leaching			
Dermal – Consumer Use			
Inhalation – Consumer Use			
RISK ASSESSMENT CALCULATIONS:			
MOE – Acute Occupational Exposure		N/A	
MOE – Chronic Occupational Exposure		5000	
MOE – Acute General Population Exposure		N/A	
MOE – Chronic General Population Exposure		3.9×10^6	

CAS No. 1330-61-6

Submitter: The Green Chemical Company

SUMMARY CONCLUSIONS:

Occupational Risk:

Risk of Non-Cancer Acute Effects from Occupational Exposure: Low potential for risk due to low hazard since mammalian LD₅₀ >50 mg/kg.

Risk of Non-Cancer Chronic Effects from Occupational Exposure: Low potential for chronic risk because MOE >1000.

Risk of Cancer Effects from Occupational Exposure: Low potential for risk since there is low hazard concern.

General Population Risk:

Risk of Non-Cancer Acute Effects to General Population: Low potential for risk due to low hazard since mammalian LD₅₀ >50 mg/kg.

Risk of Non-Cancer Chronic Effects to General Population: Low potential for chronic risk because MOE >1000.

Risk of Cancer Effects to General Population: Low potential for risk since there is low hazard concern.

Aquatic Risk:

Acute Risk to the Aquatic Environment: Low potential for acute risk because PEC does not exceed acute COC.

Chronic Risk to the Aquatic Environment: Low potential for chronic risk because PEC does not exceed chronic COC more than 20 days per year.

WRITE-UP SECTIONS:

Physical/Chemical Properties

GCC001 is a liquid at room temperature with a measured melting point of -100 °C and a measured boiling point of 158 °C at 50 mm Hg (PhysProp Database). This melting point was input into EPISuite, but the boiling point was not, since it was measured at a reduced pressure. All of the remaining physical properties were estimated by EPISuite. GCC001 is expected to be slightly soluble in water, estimated at about 3 mg/L. The estimated vapor pressure of 0.023 mm Hg indicates that the material will exist primarily in the vapor phase in the atmosphere. Due to the relatively high vapor pressure and low water solubility, material is estimated to volatilize readily from water with a Henry's Law constant of 1.2×10^{-3} atm-m³/mole.

Environmental Fate

No references to the environmental fate of GCC001 were located in the available literature, and its environmental fate is based on EPI estimates. If released to the environment, GCC001 is not expected to be persistent. In air, the estimated half-life for the gas-phase reaction with hydroxyl radicals is 17 hours. The gas-phase reaction with ozone will also contribute to its atmospheric destruction. GCC001 is not expected to undergo hydrolysis under conditions typically found in the environment, with an estimated half-life of 1 year at pH 8 and over 10 years under neutral conditions based on HYDROWIN estimates. Biodegradation is expected to be the predominant degradation process in water and soil, with ultimate biodegradation occurring within weeks, as estimated by the expert survey biodegradation model. Volatilization from water to the atmosphere is expected to be a competing process for its removal from streams based on EPI estimates. Its soil adsorption coefficient ($\log K_{oc} = 3.1$) indicates moderate adsorption to soil and slow migration to groundwater. The K_{oc} also indicates potential for adsorption to sediment and suspended organic matter in surface waters. Consistent with this assessment, the Level III fugacity model indicates that it will partition predominantly to soil, with lesser amounts to water and sediment. An estimated BCF of 161 indicates low potential to bioconcentrate in fish and aquatic organisms. GCC001 is not estimated to be a PBT based on the results of the PBT Profiler.

Overall, GCC001 is expected to partition mainly to soil and have low persistence.

CAS No. 1330-61-6

Submitter: The Green Chemical Company

Aquatic Hazard

The ecotoxicity estimates are based on structure activity relationship (SAR) equations in the ECOSAR software. In the case of GCC001, the estimates are based on the "Acrylates" SAR, and the software was able to estimate values for all three acute endpoints (fish, daphnid, and green algae) and one chronic endpoint (fish); the estimated effect levels for acute fish and daphnid are close to the log K_{ow} cutoffs for the SAR. In order to complete the aquatic toxicity profile for the 2 remaining chronic endpoints (daphnid and green algae), an acute-to-chronic ratio (ACR) was applied to the corresponding acute endpoint (10 for daphnid and 4 for green algae). In this way, effect levels for all 6 endpoints (fish acute and chronic, daphnid acute and chronic, and green algae acute and chronic) were estimated. An acute effect level value <1 mg/L indicates a high hazard concern, a value between 1 and 100 mg/L indicates a moderate hazard concern, and a value >100 mg/L indicates a low hazard concern. A chronic endpoint value <0.1 mg/L indicates a high hazard concern, between 1 and 10 indicates a moderate hazard concern, and >10 mg/L indicates a low hazard concern. A concentration of concern (COC) is estimated for both acute and chronic endpoints for each species by dividing the relevant endpoint by a factor and rounding the result to one significant digit; all results <1 μ g/L (ppb) are rounded up to 1 μ g/L. These COCs are used to determine risk (see below).

Overall, for GCC001 all three acute effect level estimates are <1 mg/L and all three chronic effect level estimates are <0.1 mg/L, indicating a high hazard concern for this chemical.

Human Health Cancer Hazard

No data were identified either on the GCC001 (isodecyl acrylate) or structural analogs that indicate a concern for carcinogenicity. Overall, there appears to be a low carcinogenicity concern for the submitted substance based on three factors: (1) OncoLogic predicted a "Marginal" concern for cancer effects; (2) an analog of the submitted substance (isooctyl acrylate) was not carcinogenic when applied dermally to male mice in an adequately conducted lifetime bioassay (Gordon et al 1991); and (3) isooctyl acrylate and hexyl acrylate produced negative results in adequately conducted mutation assays.

Based on analog data and OncoLogic predictions, GCC001 is estimated to pose a low concern for human health cancer hazard.

Human Health Non-Cancer Hazard

No relevant toxicity data for GCC001 were identified and the assessment was based on data identified for analogs. A close structural analog, isooctyl acrylate (CAS No. 29590-42-9) had low acute toxicity with a reported LD_{50} of >5000 mg/kg for rats by oral gavage (IUCLID 29590-42-9). In a separate study, isooctyl acrylate produced skeletal variations in offspring at 1000 mg/kg-day (the only dose tested) when administered to pregnant rats via oral gavage. However, isooctyl acrylate did not induce developmental toxicity when dermally administered to rats in an adequately conducted study; therefore, there does not appear to be a developmental toxicity concern when dermal exposure is expected. Dermal sensitization was also identified as a potential concern based on analogy to octyl acrylate, octyl and decyl acrylate mixture, and hexyl acrylate, all of which induced dermal sensitization reactions in either laboratory animals or human volunteers. Table 1 reports the potential hazard concerns identified for selected analogs of the submitted substance.

Based on developmental effects for a close structural analog at 1000 mg/kg-day, an overall non-cancer hazard concern of moderate was estimated for GCC001.

Environmental (Aquatic) Exposure

Environmental exposure may result from releases of GCC001 to surface water from a single site during cleaning of the reactor, which occurs 1 day/year. ChemSTEER estimates a release of 11.2 kg/site-day to surface waters, with total releases of 11.2 kg/year. The aquatic exposure estimates indicate a predicted environmental concentration (PEC) of 2.82 µg/L (E-FAST). The PEC and the days per year of release will be used to determine risk potential to the aquatic environment resulting from releases of GCC001.

Occupational Exposure

Occupational exposures were estimated using ChemSTEER. Based on the expected use and manufacturing of the submitted chemical, workers may be exposed to vapors (inhalation exposure) at up to 2.59 mg/day (10 days/year) and to liquid (dermal exposure) at up to 441 mg/day (10 days/year) from loading liquid product into drums. These daily exposures are used by ChemSTEER to estimate lifetime average daily dose rates (LADD), average daily dose rates (ADD), and acute potential dose rates (APDR) for both inhalation and dermal exposure to GCC001. The calculated dose rates are listed on the exposure models page above. Potential risk to workers will be calculated by comparison of the appropriate exposure value, assuming that no protective gear is used, to the estimated LOAEL of 1000 mg/kg-day and is discussed in the following section.

General Population Exposure

Occupational exposures were estimated using ChemSTEER. Based on expected processing of the submitted chemical, workers may be exposed to vapors (inhalation exposure), at up to 13.9 mg/day, and to liquid (dermal exposure), at up to 529 mg/day, from loading liquid product into drums, which occurs 10 days/year. These daily exposures are used by ChemSTEER to estimate lifetime average daily dose (LADD), average daily dose rates (ADD), and acute potential dose rates (APDR) for both inhalation and dermal exposure to GCC001. The calculated dose rates are listed on the exposure models page above. Potential risk to workers will be calculated by comparison of the appropriate exposure value, assuming that no protective gear is used, to the estimated LOAEL of 1000 mg/kg-day and is discussed in the following section.

Environmental (Aquatic) Risk Assessment

Acute risk to the aquatic environment is estimated by comparison of the acute COC for each species to the estimated PEC (see Appendix 1 below). If the PEC > the acute COC estimated for a species, then the potential for acute risk exists for that species. For GCC001, the PEC < the acute COC, indicating a low potential for acute risk to aquatic organisms.

Chronic risk to the aquatic environment is evaluated by estimating the number of days the PEC exceeds the chronic COC for each species (see Appendix 1 below). This estimation is done by E-FAST and is based on the PEC, the number of days of release per year, and estimated stream flow rates. If the PEC is estimated to exceed the relevant chronic COC for 20 days/year or more, a potential for chronic risk exists for the species being evaluated. GCC001 is estimated to have releases to the aquatic environment for 1 day/year and, in all cases, the PEC exceeds the COC for < 20 days/year, indicating a low potential for chronic risk to the aquatic environment.

Overall, GCC001 is estimated to pose a low potential for acute and chronic risk to the environment.

Human Health Risk Assessment

Risk is assessed by establishing a margin of exposure (MOE) for both occupational exposure and general population exposure for each relevant effect estimated for the chemical. This is done by dividing the effect level, either a lowest-observed-adverse-effect level (LOAEL) or a no-observed-adverse-effect level (NOAEL), by the estimated exposure dose. In the case of a LOAEL, a MOE <1000 indicates a potential for risk for that effect from that exposure; in the case of an NOAEL, a MOE <100 indicates potential for risk. For GCC001, developmental toxicity is based on analogy to isooctyl acrylate, which induced skeletal variations at 1,000 mg/kg-day; a NOAEL was not observed. Developmental effects are systemic or chronic effects that are caused by acute exposure of a pregnant female. The LOAEL for this effect is compared to the highest relevant acute dose rate (APDR and ADRpot) for both occupational exposure and general population exposure. In the case of occupational exposure, the inhalation APDR is used, even though the dermal APDR is higher, since the study specifically showed that dermal exposure does not induce developmental effects. If effect levels, either LOAELs or NOAELs, were estimated for multiple effects shown in the table above, each would be subject to risk assessment, as described, using the relevant potential exposure levels.

Cancer human health risk assessment is not currently performed for a Sustainable Futures summary assessment; however, in cases where there is low hazard concern for human health cancer effects, there will be low risk for cancer effects also.

Risk from occupational exposure is estimated by dividing the estimated LOAEL of 1000 mg/kg-day by the inhalation APDR of 0.199 mg/kg-day to get the MOE (see Appendix 2 below). The MOE from this calculation is >1000 (5000), indicating a low potential for risk from occupational exposure to GCC001.

Risk to the general population is estimated by dividing the LOAEL of 1000 mg/kg-day by the fish ingestion ADRpot of 2.56×10^{-4} mg/kg-day, which represents the source of general population exposure with the highest potential exposure level, to get the MOE (see Appendix 3 below). The MOE from this calculation is >1000 (3.9×10^6), indicating a low potential for risk to the general population from exposure to GCC001.

Overall, GCC001 has a low potential for risk to human health from occupational exposure and general population exposure.

Abbreviations Used

GCC001 – Chemical and assessment ID (isodecyl acrylate)

SAR – Structure activity relationship

ACR – Acute-to-chronic ratio

COC – Concentration of concern

PEC – Predicted environmental concentration

LADD/LADDpot – Lifetime average daily dose (potential)

ADD /ADDpot – Average daily dose (potential)

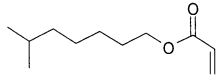
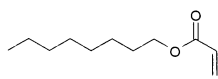
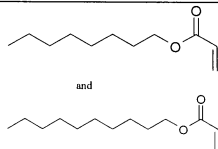
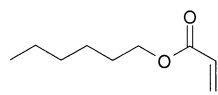
APDR/ADRpot – acute potential dose rate

MOE – margin of exposure

CAS No. 1330-61-6

Submitter: The Green Chemical Company

Table I - Selected Analogs

Analogue	Structure	Concern Identified	Basis of Concern	Concern Level
Isooctyl acrylate (29590-42-9) TSCATS 8-e-1524, 8e-3774; (IUCLID 29590-42-9)		<u>Positive:</u> Developmental toxicity (oral), dermal sensitization, dermal irritation <u>Negative:</u> Developmental toxicity (dermal), genotoxicity, cancer (dermal), acute toxicity	Induced skeletal variations at 1000 mg/kg-day (only dose tested) in rats by oral gavage; Acute LD ₅₀ of >5000 mg/kg in rats by oral gavage; Skin irritation in rabbits	Moderate for developmental effects; Low for acute toxicity; N/A for skin irritation
Octyl acrylate (2499-59-4) TSCATS 8(e)-1572		<u>Positive:</u> Dermal sensitization	Induced skin sensitization in laboratory animals	N/A
Octyl and decyl acrylate mixture TSCATS 8(e)-11424		<u>Positive:</u> Dermal sensitization	Produced positive results in mouse ear swelling test	N/A
Hexyl acrylate (2499-95-8) TSCATS 8(e)-3774 CCRIS		<u>Positive:</u> Dermal sensitization (6% solution) <u>Negative:</u> Genotoxicity	Induced skin sensitization in human volunteers	N/A

References

CCRIS. Chemical Carcinogenesis Research Information System. 2004. Available on-line at <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS>

Gordon, S.C.; Zimmerman, D.D.; and F.D. Griffith. 1991. Acute Toxicity, Genotoxicity, and Dermal Carcinogenicity Assessment of Isooctylacrylate. *J Toxicol Environ Health*. 34(3)297-308.

IUCLID 29590-42-9. IUCLID data sheet for isooctyl acrylate, CAS No. 29590-42-9.

TSCA Section 8(e) submission, 8(e)-1524. TSCATS Database. Teratology Screen in Rats (C190, C-181, C-183, C-236, C-253, C-254, C-255, C-256, C-257, C-258, C-259) (Final Report) with attachments and cover letter. U.S.EAP/OPTS Public Files: Fiche#: OTS0534620, Doc#: 88-920000170.

TSCA Section 8(e) submission, 8(e)-11424. TSCATS Database. Initial Submission: Mouse ear swelling test with octyl decyl acrylate with cover letter dated 102792; U.S. EPA/OPTS Public Files: Fiche#: OTS0571362, Doc#: 88-920009705.

TSCA Section 8(e) submission, 8(e)-14572. TSCATS Database. Initial Submission: Acrylate de n-octyle, Skin sensitization test in guinea pigs (Maximization method of Magnusson, B. and Kligman, A.M.), with cover letter dated 101599; U.S. EPA/OPTS Public files: Fiche#: OTS0559819, Doc#: 88-000000012.

TSCA Section 8(e) submission, 8(e)-3774. TSCATS Database. Initial Submission: Letter concerning information on the chemical substance hexyl acrylate with attachments (SANITIZED); U.S. EPA/OPTS Public Files: Fiche#: OTS0536468, Doc#: 88-9200024168.

Appendix 1: Determination of Aquatic Risk

Chemical Identifier: GCC001

CAS Number: 1330-61-6

Release Activity 1: User-Defined Processing **Site Information:** Adhesives and Sealants Processing

	Endpoint	Effect Level (ppb)	Assessment Factor	Acute COC (ppb)	PEC (ppb)	Potential for Risk?
Acute Profile	Fish	900	5	200	2.82	No
	Daphnid	550	5	100	2.82	No
	Green Algae	70	4	20	2.82	No
Chronic Profile	Endpoint	Effect Level (ppb)	Assessment Factor	Chronic COC (ppb)	Days/Year PEC Exceeds COC	Potential for Risk?
	Fish	5	10	1	<1	No
	Daphnid	60	10	6	<1	No
	Green Algae	20	10	2	<1	No

Appendix 2: Determination of Human Health Risk from Occupational Exposure

Chemical Identifier: GCC001

CAS Number: 1330-61-6

Exposure Activity 1: User-Defined Processing **Site Information:** Adhesives and Sealants Processing

	Endpoint (Concern Effect)	NOAEL (mg/kg-d)	LOAEL (mg/kg-d)	Exposure Dose and Source (mg/kg-d)	MOE*	Potential for Risk?
Occupational Exposure	1. Developmental Effects		1000	0.199 (inhalation APDR)	5000	No
	2.					
	3.					

*MOE < 100 indicates potential for risk when using a NOAEL value; MOE < 1000 indicates potential for risk when using a LOAEL value.

Appendix 3: Determination of Human Health Risk to the General Population

Chemical Identifier: GCC001

CAS Number: 1330-61-6

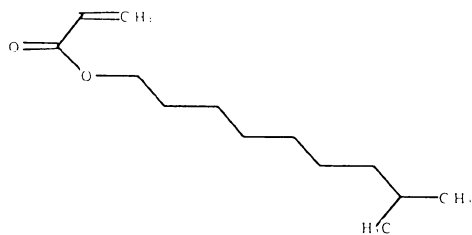
Exposure Activity 1: User-Defined Processing Site Information: Adhesives and Sealants Processing

	Endpoint (Concern Effect)	NOAEL (mg/kg-d)	LOAEL (mg/kg-d)	Exposure Dose and Source (mg/kg-d)	MOE*	Potential for Risk?
General Population Exposure	1. Developmental Effects		1000	2.56×10^{-4} (Fish Ingestion Acute ADRpot)	3.9×10^6	No
	2.					
	3.					

*MOE < 100 indicates potential for risk when using a NOAEL value; MOE < 1000 indicates potential for risk when using a LOAEL value.

Attachment 3

EPIWIN (EPISuite): Physicochemical Properties/Environmental Fate



SMILES : O=C(C=C)OCCCCCCCC(C)C
 CHEM : 2-Propenoic acid, isodecyl ester
 CAS NUM: 001330-61-6
 MOL FOR: C13 H24 O2
 MOL WT : 212.34

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

Physical Property Inputs:

Water Solubility (mg/L): -----
 Vapor Pressure (mm Hg) : -----
 Henry LC (atm-m3/mole) : -----
 Log Kow (octanol-water): -----
 Boiling Point (deg C) : -----
 Melting Point (deg C) : -100.00

Log Octanol-Water Partition Coef (SRC):
 Log Kow (KOWWIN v1.67 estimate) = 5.07

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
 Boiling Pt (deg C): 253.36 (Adapted Stein & Brown method)
 Melting Pt (deg C): 11.48 (Mean or Weighted MP)
 VP (mm Hg, 25 deg C): 0.0227 (Mean VP of Antoine & Grain methods)
 MP (exp database): -100 deg C
 BP (exp database): 158 @ 50 mm Hg deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):
 Water Solubility at 25 deg C (mg/L): 3.034
 log Kow used: 5.07 (estimated)
 melt pt used: -100.00 deg C

Water Sol Estimate from Fragments:
 Wat Sol (v1.01 est) = 2.3895 mg/L

ECOSAR Class Program (ECOSAR v0.99h):
 Class(es) found:
 Acrylates

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
 Bond Method : 1.18E-003 atm-m3/mole
 Group Method: 1.20E-003 atm-m3/mole
 Henrys LC [VP/WSol estimate using EPI values]: 2.090E-003 atm m3/mole

Probability of Rapid Biodegradation (BIOWIN v4.02):
 Biowin1 (Linear Model) : 0.8206
 Biowin2 (Non-Linear Model) : 0.9833
 Expert Survey Biodegradation Results:
 Biowin3 (Ultimate Survey Model): 2.8701 (weeks)
 Biowin4 (Primary Survey Model) : 3.7703 (days)
 Readily Biodegradable Probability (MITI Model):
 Biowin5 (MITI Linear Model) : 0.7388
 Biowin6 (MITI Non-Linear Model): 0.8668
 Ready Biodegradability Prediction: YES

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

OVERALL OH Rate Constant = 22.2422 E-12 cm³/molecule-sec
Half-Life = 0.481 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 5.771 Hrs

Ozone Reaction:

OVERALL Ozone Rate Constant = 0.175000 E-17 cm³/molecule-sec
Half-Life = 6.549 Days (at 7E11 mol/cm³)

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Kcc : 1330
Log Koc: 3.124

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

Total Kb for pH > 8 at 25 deg C : 2.071E-002 L/mol-sec
Kb Half-Life at pH 8: 1.061 years
Kb Half-Life at pH 7: 10.607 years

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

Log BCF = 2.207 (BCF = 161.1)
log Kow used: 5.07 (estimated)

Volatilization from Water:

Henry LC: 0.0012 atm-m³/mole (estimated by Group SAR Method)
Half-Life from Model River: 2.198 hours
Half-Life from Model Lake : 146.2 hours (6.09 days)

Removal In Wastewater Treatment:

Total removal: 82.34 percent
Total biodegradation: 0.62 percent
Total sludge adsorption: 75.28 percent
Total to Air: 6.44 percent
(using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment (recommended maximum 99%):

Total removal: 99.94 percent
Total biodegradation: 79.78 percent
Total sludge adsorption: 20.05 percent
Total to Air: 0.10 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.23	10.8	1000
Water	12.9	360	1000
Soil	68.8	720	1000
Sediment	17.1	3.24e+003	0

Persistence Time: 502 hr

Attachment 4

PBT Profiler: Environmental Fate/Distribution

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
[Home](#) · [Start a New Profile](#) · [Results](#) · [Terms of Use](#) · [Security](#)

Results

Italicized or **underlined** highlights indicate that the EPA criteria have been exceeded.
[Color version](#)

Persistence

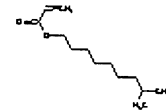
Bioaccumulation

Toxicity

1330-61-6 2-Propenoic acid, isodecyl ester

PBT Profiler Estimate = **p b I**

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	15	■ 13%	160	<u>0.005</u>
Soil	30	■ 68%		
Sediment	140	■ 17%		
Air	0.67	■ 2%		



P2 Considerations and more information

Based on its structure, this chemical may belong to the acrylates/methacrylates category. Members of this category may have potential human health concerns. [More information and category definitions.](#)

[Start a New Profile](#)

[Add More Chemicals to Your Profile](#)

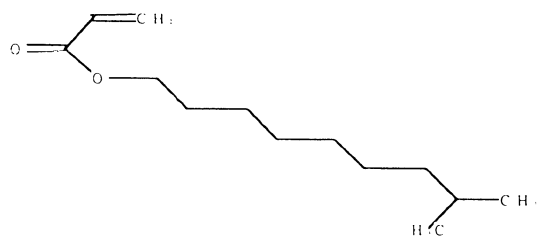
The PBT Profiler Results are available for 20 minutes

Developed by the Environmental Science Center under contract to the Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency

Computer Resources Donated by Syracuse Research Corporation Ver 1.203 Last Updated August 27, 2004

Attachment 5

ECOSAR: Aquatic Toxicity QSAR



SMILES : C=C(C=O)OCCCCCCCC(C)C
 CHEM : 2-Propenoic acid, isodecyl ester
 CAS Num: 001330-61-6
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C13 H24 O2
 MOL WT : 212.34
 Log Kow: 5.07 (KowWin estimate)
 Melt Pt: 25.00 deg C
 Wat Sol: 2.222 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

 Acrylates

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.604
Acrylates	: Fish	96-hr	LC50	0.900
Acrylates	: Daphnid	48-hr	LC50	0.554
Acrylates	: Green Algae	96-hr	EC50	0.066
Acrylates	: Fish	32-day	ChV	0.005

Note: * - asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
 Fish and daphnid acute toxicity log Kow cutoff: 5.0
 Green algal EC50 toxicity log Kow cutoff: 6.4
 Chronic toxicity log Kow cutoff: 8.0
 MW cutoff: 1000

Attachment 6

OncoLogic: Carcinogenicity Potential SAR

OncoLogic Justification Report

SUMMARY:

CODE NUMBER: case1

SUBSTANCE ID: case1

The final level of carcinogenicity concern for this acrylate when the anticipated route of exposure is inhalation or injection is MARGINAL.

The final level of carcinogenicity concern for this acrylate when the anticipated route of exposure is oral or dermal is LOW.

JUSTIFICATION:

An acrylate is a potential alkylating agent which may bind, via Michael addition, to key macromolecules to initiate/exert carcinogenic action. The alkylating activity of acrylates can be substantially inhibited by substitution at the double bond, particularly by bulky or hydrophilic groups. The nature and molecular size/shape of the molecule to which the acrylate is attached may also play a role in affecting the overall activity of the compound.

The acrylate is stable and has a baseline level of concern of LOW-MODERATE.

The molecule to which the acrylate is attached, which is denoted as R1, is expected to reduce the level of concern.

Therefore, the level of concern is reduced to LOW.

In general, inhalation and injection provide the best chance of delivering the largest possible amount of direct-acting reactive chemicals to target tissue because of a lesser absorption barrier and better chance of avoiding detoxification by protective nucleophiles such as glutathione. Exposure to the compound by either of these routes is expected to raise the level of concern to MARGINAL.

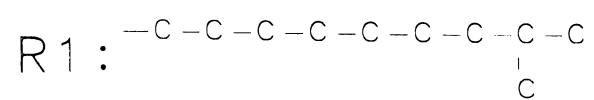
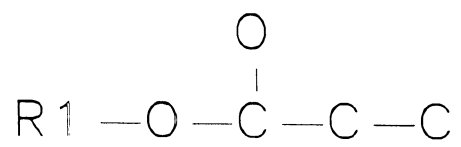
Exposure by the oral and dermal routes is not expected to significantly affect the level of concern, therefore the level of concern remains LOW.

The final level of concern when the anticipated route of exposure is inhalation or injection is MARGINAL.

The final level of concern when the anticipated route of exposure is oral or dermal is LOW.

Compound Display

CASE 1



Attachment 7

**ChemSTEER: Occupational Exposure & Environmental
Release**

3/15/2005

INITIAL REVIEW ENGINEERING REPO CBI: No
ID Number: Case Study

ENGINEER: Thomas webb \
PV (kg/yr): 11,200.00 Import
SUBMITTER: The Green Chemical Corporation

USE: Reactive diluent in UV/EB curable
coatings and adhesives.

OTHER USES:

MSDS: No Label: No

Gen Eqpt: gloves/goggles/glasses/local
exhaust ventilation/general mechanical
ventilation/other (please specify):
Respirator: air purifying/organic
vapor/dust/paint mist/supplied air/other
(please specify):
Health Effects: corrosive/flammable/other
(please specify):

TLV/PEL:

CRSS:
Chemical Name: Isodecyl acrylate
Chemical Category: Acrylate
S-H2O: 0.00303 g/L @ 25.00
VP: 0.0227000010 torr @ 25.00
MW: 212.34 %<500 %<1000
Phys State
NEAT:
Out of User-defined Processing: Solution

Consumer Use: No

SAT
(concerns):
Related cases:
Migration to groundwater:
PBT rating: PBT
Health:
Eco:

OCCUPATIONAL EXPOSURE RATING:

NOTES & KEY ASSUMPTIONS:

POLLUTION PREVENTION CONSIDERATIO

EXPOSURE-BASED REVIEW: No (0 criteria met)
1) # of workers exposed: >1000? No
2) >100 workers with >10 mg/day inhalation
exposure: No
3) (a) >100 workers w/1-10 mg/day inh. exp. &
>100 days/yr: No
(b) Routine Dermal Cont: >250 workers &
Page 1

>100 days/yr: No

----- page break -----

3/15/2005
INITIAL REVIEW ENGINEERING REPORT
CBI: No

ID Number: Case Study
User-defined Processing
Number of Sites: 1

Days/yr: 10
Basis:

Process Description:

ENVIRONMENTAL RELEASES ESTIMATE SUMMARY

Air
4.3040E-03 kg/site-day over 1 days/yr
from: Equipment Cleaning Losses of Liquids
from a Single, Large Vessel; Loading Liquid
Product into Drums
basis: EPA/OPPT Mass Transfer Coefficient
Model.; EPA/OAQPS AP-42 Loading Model.

Air
9.6848E-04 kg/site-day over 9 days/yr
from: Loading Liquid Product into Drums
basis: EPA/OAQPS AP-42 Loading Model.

Water
11.2 kg/site-day over 1 days/yr
from: Equipment Cleaning Losses of Liquids
from a Single, Large Vessel
basis: EPA/OPPT Single Vessel Residual Model,
CEB standard 1% residual.

OCCUPATIONAL EXPOSURES ESTIMATE SUMMARY
Tot. # of workers: 1

Inhalation:

Exposure to Vapor
13.9353 mg/day over 10 days/yr
Number of workers (all sites) with inhalation
basis: Loading Liquid Product into Drums;
EPA/OPPT Mass Balance Model.

Dermal:

Exposure to Liquid at 30.00% concentration
529.20 mg/day over 10 days/yr
Number of workers (all sites) with dermal expo
basis: Loading Liquid Product into Drums;
EPA/OPPT 2-Hand Dermal Contact with Liquids
Model.

Attachment 8

E-FAST: Aquatic & General Population Exposure

INITIAL REVIEW EXPOSURE REPORT

Case Number: Case Study Assessor:

ENVIRONMENTAL RELEASES

Scenario#: 1 Number of Release Sites: 1.

Release Activity: Processing

Release Description:	WATER	LANDFILL	INCINER	LAND/INCIN	FUGITIVE
Total Releases:	11.20 (kg/yr)	0.00 (kg/yr)	0.00 (kg/yr)	0.00 (kg/yr)	9.70E-03 (kg/yr)
Release Days/yr:	1.				10.
Per Site Release:	11.20 (kg/day)	0.00 (kg/yr)	0.00 (kg/yr)	0.00 (kg/yr)	9.70E-04 (kg/day)
Remarks:					

INITIAL REVIEW EXPOSURE REPORT

CASE NUMBER: Case Study

SIC-CODE BASED HUMAN AND AQUATIC EXPOSURES TO SURFACE WATER RELEASES

SCENARIO #: 1

RELEASE ACTIVITY: Processing

SIC-CODE DESCRIPTION: Adhesives and Sealants Manufacture

SIC-CODE (S): 2891

EXPOSED POPULATION:

WASTE WATER TREATMENT REMOVAL (%)	RELEASE DAYS	PRE-TREATMENT RELEASE (kg/day)	POST-TREATMENT RELEASE (kg/day)	BCF (L/kg)
99.	1.	11.2	0.11	161.00

AQUATIC EXPOSURE ESTIMATES - SURFACE WATER

PLANT TYPE	% ILE FACILITY	STREAM FLOW (MLD)				STREAM CONC. (µg/l)			
		Harmonic MEAN	30Q5	7Q10	1Q10	Harmonic MEAN	30Q5	7Q10	1Q10
ALL	50	1144.60	390.56	264.95	214.80	9.79E-02	0.29	0.42	0.52
ALL	10	126.44	62.49	39.74	32.65	0.89	1.79	2.82	3.43

DRINKING WATER INGESTION EXPOSURE ESTIMATES (50%ile facility)

Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	IR (L/day)
Cancer					
LADD _{pot} (mg/kg/day)	2.09E-09	30.00	75.00	71.80	1.40
LADC _{pot} (mg/L)	1.07E-07	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	5.23E-09	30.00	30.00	71.80	1.40
ADC _{pot} (mg/L)	2.68E-07	30.00	30.00	NA	NA
Acute					
ADR _{pot} (mg kg/day)	2.40E-05	1.00 day	1.00 day	71.80	6.00

INITIAL REVIEW EXPOSURE REPORT

CASE NUMBER: Case Study

SIC-CODE BASED HUMAN AND AQUATIC EXPOSURES TO SURFACE WATER RELEASES (CONT.)

FISH INGESTION EXPOSURE ESTIMATES (50%ile facility)					
Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	IR (g/day)
Cancer					
LADD _{pot} (mg/kg/day)	1.44E-09	30.00	75.00	71.80	6.00
LADC _{pot} (mg/kg)	1.73E-05	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	3.61E-09	30.00	30.00	71.80	6.00
ADC _{pot} (mg/kg)	4.32E-05	30.00	30.00	NA	NA
Acute					
ADR _{pot} (mg/kg/day)	2.83E-05	1.00 day	1.00 day	71.80	129.00

DRINKING WATER INGESTION EXPOSURE ESTIMATES (10%ile)					
Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	IR (L/day)
Cancer					
LADD _{pot} (mg/kg/day)	1.89E-08	30.00	75.00	71.80	1.40
LADC _{pot} (mg/L)	9.71E-07	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	4.73E-08	30.00	30.00	71.80	1.40
ADC _{pot} (mg/L)	2.43E-06	30.00	30.00	NA	NA
Acute					
ADR _{pot} (mg/kg/day)	1.50E-04	1.00 day	1.00 day	71.80	6.00

SIC-CODE BASED HUMAN AND AQUATIC EXPOSURES TO SURFACE WATER RELEASES (CONT.)

FISH INGESTION EXPOSURE ESTIMATES (10%ile facility)					
Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	IR (g/day)
Cancer					
LADD _{pot} (mg/kg/day)	1.31E-08	30.00	75.00	71.80	6.00
LADC _{pot} (mg/kg)	1.56E-04	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	3.27E-08	30.00	30.00	71.80	6.00
ADC _{pot} (mg/kg)	3.91E-04	30.00	30.00	NA	NA
Acute					
ADR _{pot} (mg/kg/day)	2.56E-04	1.00 day	1.00 day	71.80	129.00

INITIAL REVIEW EXPOSURE REPORT

CASE NUMBER: Case Study

SIC CODE EXPOSURES TO SURFACE WATER RELEASES

SCENARIO #: 1

RELEASE ACTIVITY: Processing

SIC CODE DESCRIPTION: Adhesives and Sealants Manufacture

ASSOCIATED SIC CODES: 2891

SIC CODE RESULTS

COC ($\mu\text{g/L}$)	% yr exceeded	Days/yr exceeded	Release days/year	Loading (kg/site/day)	Waste Water Treatment (%)	High/Avg Analysis
1.00	0.11	0.39	1.00	11.20	99.00	High

INITIAL REVIEW EXPOSURE REPORT

CASE NUMBER: Case Study

INHALATION EXPOSURE ESTIMATES FROM FUGITIVE RELEASES

SCENARIO #: 1

RELEASE ACTIVITY: Processing

RELEASE DESCRIPTION:

METHOD OF CALCULATION: Turner

EXPOSED POPULATION:

NUMBER OF SITES	% TREATMENT	TYPE OF REMOVAL	PRE-TREAT RELEASE (kg/yr)	POST-TREAT RELEASE (kg/yr)
1.	0.00	None	9.70E-03	9.70E-03

Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	Inh. Rate (m ³ /hr)
Cancer					
LADD _{pot} (mg/kg/day)	9.77E-11	30.00	75.00	71.80	0.55
LADC _{pot} (mg/m ³)	1.94E-08	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	2.44E-10	30.00	30.00	71.80	0.55
ADC _{pot} (mg/m ³)	4.85E-08	30.00	30.00	NA	NA

INITIAL REVIEW EXPOSURE REPORT

Case Number: Clean Assessor:

ENVIRONMENTAL RELEASES

Scenario#: 1 Number of Release Sites: 1.

Release Activity: Processing

Release Description:	WATER	LANDFILL	INCINER	LAND/INCIN	FUGITIVE
Total Releases:	0.00	0.00	0.00	0.00	3.34E-03
	(kg/yr)	(kg/yr)	(kg/yr)	(kg/yr)	(kg/yr)
Release Days/yr:	0.				1.
Per Site Release:	0.00	0.00	0.00	0.00	3.34E-03
	(kg/day)	(kg/yr)	(kg/yr)	(kg/yr)	(kg/day)

Remarks:

INITIAL REVIEW EXPOSURE REPORT

CASE NUMBER:Clean

INHALATION EXPOSURE ESTIMATES FROM FUGITIVE RELEASES

SCENARIO #:1

RELEASE ACTIVITY:Processing

RELEASE DESCRIPTION:

METHOD OF CALCULATION:Turner

EXPOSED POPULATION:

NUMBER OF SITES	% TREATMENT	TYPE OF REMOVAL	PRE-TREAT RELEASE (kg/yr)	POST-TREAT RELEASE (kg/yr)
1.	0.00	None	3.34E-03	3.34E-03

Exposure Units	Results	ASSUMPTIONS			
		ED (years)	AT (years)	BW (kg)	Inh. Rate (m ³ /hr)
Cancer					
LADD _{pot} (mg/kg/day)	3.36E-12	30.00	75.00	71.80	0.55
LADC _{pot} (mg/m3)	6.68E-09	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADD _{pot} (mg/kg/day)	8.41E-12	30.00	30.00	71.80	0.55
ADC _{pot} (mg/m3)	1.67E-08	30.00	30.00	NA	NA