

201-15031A

2-Propenoic Acid, Isodecyl Ester

(Isodecyl Acrylate; CAS RN 1330-61-6)

**High Production Volume (HPV) Chemical
Challenge Test Plan and Data Review**

Prepared for:

ACC Specialty Acrylates and Methacrylates Panel

Prepared by:

Toxicology/Regulatory Services, Inc.

RECEIVED
OPPT/DBIC
04 JAN 12 PM 3:08

December 2003

2-Propenoic Acid, Isodecyl Ester
High Production Volume Chemical Challenge
Test Plan and Data Review

Table of Contents		<u>Page</u>
1.0	Introduction.....	4
2.0	General Use and Exposure.....	4
3.0	Justification for Use of Isooctyl Acrylate (IOA) Data to Support Isodecyl Acrylate.....	4
4.0	General Substance Information (Identity)	5
5.0	Physical/Chemical Properties	6
5.1	Melting Point	6
5.2	Boiling Point	6
5.3	Vapor Pressure	6
5.4	Partition Coefficient.....	6
5.5	Water Solubility	6
6.0	Environmental Fate.....	7
6.1	Photodegradation	7
6.2	Water Stability	7
6.3	Transport and Distribution.....	7
6.4	Biodegradability.....	8
7.0	Ecotoxicity	8
7.1	Toxicity to Fish.....	8
7.2	Toxicity to Aquatic Invertebrates	8
7.3	Toxicity to Aquatic Plants	8
7.4	Chronic Toxicity to Aquatic Invertebrates	9
8.0	Human Health-Related Data	9
8.1	Acute Toxicity	9
8.2	Repeated Dose Toxicity.....	9
8.3	Genetic Toxicity.....	9
8.3.1	<i>In vitro</i>	9
8.4	Reproductive and Developmental Toxicity	10
9.0	Conclusion	10
10.0	References.....	11

Tables

	<u>Page</u>
Test Plan	4
Table 1: Data Summary	14

Test Plan

2-Propenoic Acid, Isodecyl Ester (Isodecyl Acrylate; CAS RN: 1330-61-6)		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
IUCLID #	PHYSICAL AND CHEMICAL DATA							
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapor Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	N	N	Y	Y	Y	N
IUCLID #	ENVIRONMENTAL FATE AND PATHWAY							
3.1.1	Photodegradation	Y	N	N	N	Y	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.3	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	Y	N	N	N	Y	N
IUCLID #	ECOTOXICITY							
4.1	Acute Toxicity to Fish	Y	Y	N	N	N	Y	N
4.2	Toxicity to Daphnia	Y	Y	N	N	N	Y	N
4.3	Acute Toxicity to Algae	Y	Y	N	N	N	Y	N
IUCLID #	TOXICITY							
5.1	Acute Toxicity	Y	Y	Y	N	N	Y	N
5.4	Repeated Dose Toxicity	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Bacterial Test)	Y	Y	N	N	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Mammalian Cells)	Y	Y	Y	N	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	Y	Y	N	N	Y	N

**2-Propenoic Acid, Isodecyl Ester
(Isodecyl Acrylate; CAS RN 1330-61-6)
High Production Volume Chemical Challenge
Test Plan and Data Review**

1.0 Introduction

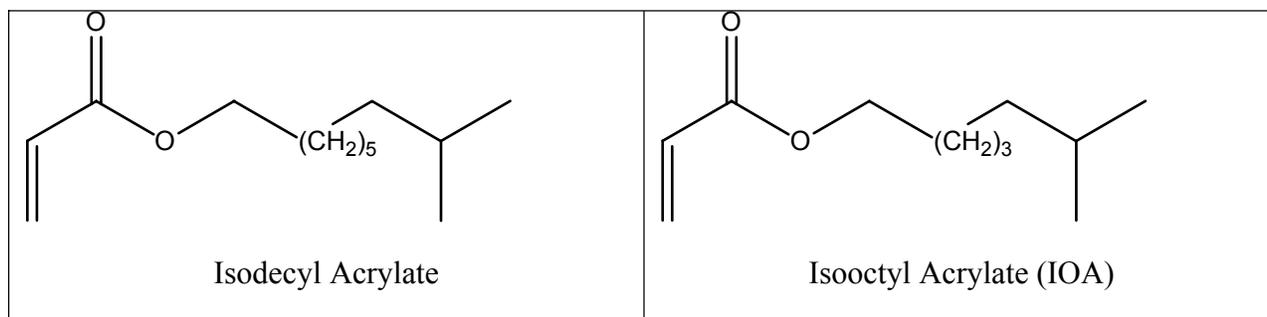
This document provides a Test Plan and reviews the data availability for the High Production Volume (HPV) Chemical Challenge Program (Program) endpoints for 2-Propenoic Acid, Isodecyl Ester, hereafter called Isodecyl Acrylate [CAS RN 1330-61-6], for the American Chemistry Council's Specialty Acrylates and Methacrylates Panel. The availability of adequate data applicable to Isodecyl Acrylate for Program endpoints is summarized in the Test Plan table.

2.0 General Use and Exposure

Isodecyl Acrylate is manufactured as an intermediate used for the synthesis of acrylic polymers. Applications include wood and vinyl coatings for floorings, pressure sensitive adhesives, paper coatings, release coatings, optical coatings and screen inks. Isodecyl Acrylate is used in ultraviolet and electron beam (UV/EB) curing processes for production of polymers. UV/EB processes are low-energy technologies that eliminate or greatly reduce the need for volatile organic solvents. In addition, curing rates are very rapid and the reactions virtually complete such that residual monomer is negligible in the final product. Occupational exposure may occur either as the liquid or vapor. Ventilation systems are used to limit vapor exposure. Air monitoring studies reported in the SIAR for the closely related isooctyl acrylate (IOA), for processing and manufacturing areas have typically indicated airborne concentrations to be below the limit of detection. Since Isodecyl Acrylate is slightly less volatile than IOA, inhalation exposure to workers is not anticipated. Federal regulations require impermeable gloves to be worn by all employees who may come into contact with unreacted monomer. Based on the high cross-linking and very low residual monomer in finished products, consumer exposure to Isodecyl Acrylate is not anticipated.

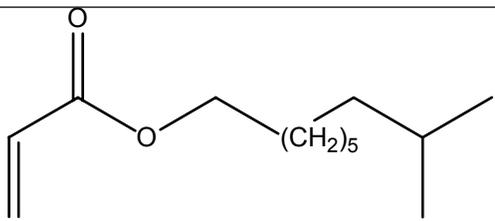
3.0 Justification for Use of Isooctyl Acrylate (IOA) Data to Support Isodecyl Acrylate

Isodecyl Acrylate and Isooctyl Acrylate (CAS number 29590-42-9), hereafter referred to as IOA, are very similar congeners of a large family of closely related acrylic acid esters. They are comprised of long-chain hydrocarbon esters with terminal branching. The two chemicals are hydrophobic and similar in general physical/chemical and toxicological properties, and belong to the larger category of physically and toxicologically similar chemicals known as the Specialty Acrylates and Methacrylate Category. The structures of these two acrylate esters are shown below.



The Organization for Economic Cooperation and Development (OECD) has completed a Screening Information Data Set (SIDS) assessment on IOA (SIDS, Volume 1, Part 2) and key studies for HPV Program endpoints are summarized in the SIDS Initial Assessment Report (SIAR) for IOA that accompanies this Test Plan. The OECD evaluation concluded: “Based on its low occupational exposure potential, its low toxicity in in vitro and mammalian studies, its limited release to the environment and its predicted rapid environmental biodegradation, IOA is considered a low priority for additional human health or environmental effects testing at this time.” As shown below and throughout this document, the physical/chemical properties, use patterns, potential environmental releases, and worker safety procedures are essentially the same for Isodecyl Acrylate and IOA. Therefore, this HPV Program test plan uses IOA data extensively in support of the HPV/SIDS endpoints for Isodecyl Acrylate.

4.0 General Substance Information (Identity)

Chemical Name	2-Propenoic Acid, Isodecyl Ester
Synonyms	Acrylic acid, Isodecyl ester Isodecyl acrylate Isodecyl alcohol, acrylate Isodecyl propenoate
CAS Number	1330-61-6
Structure	
Molecular Weight	212.32
Substance Type	Organic
Physical State	Clear Liquid

5.0 Physical/Chemical Properties

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

5.1 Melting Point

The melting point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2000a) is -100° C. No data were included in the accepted SIAR for IOA. The EPIWIN estimated melting point for Isodecyl Acrylate and IOA is 11.5 and -10.4 °C, respectively. These data are considered adequate to meet the HPV Program requirements.

5.2 Boiling Point

The boiling point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2000a) is 158 °C. The boiling point accepted in the SIAR for IOA is 196.8 °C. The EPIWIN estimated boiling point for Isodecyl Acrylate and IOA is 253.4 and 216.9 °C, respectively. The determination of the boiling point of IOA, Isodecyl Acrylate and other mono- and multi-functional acrylates is of minimal value. The double bond in these chemicals is so reactive that boiling them at atmospheric pressure results in polymerization and decomposition. As a result, these substances are not boiled at atmospheric pressure in normal manufacture or use. Moreover, distillation under vacuum at a lower temperature would generate a pure substance, since the inhibitor would be left behind. Without an inhibitor present, the pure substances quickly polymerize, even at room temperature. Therefore, the available data are considered adequate to meet the HPV Program requirements.

5.3 Vapor Pressure

The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000a) estimate vapor pressure value for Isodecyl Acrylate is 0.03 hPa. The vapor pressure accepted in the SIAR for IOA is 1.33 hPa at 25 °C and the model predicts a vapor pressure of 0.2 hPa. The value of 0.03 hPa is consistent with the large size and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

5.4 Partition Coefficient

The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000b) estimate for the log K_{ow} value of Isodecyl Acrylate is 5.07 hPa. The log K_{ow} accepted in the SIAR for IOA is 3.93, and the model predicts a log K_{ow} value of 4.09. The value of 5.07 is consistent with the hydrophobicity and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

5.5 Water Solubility

The reported value for water solubility of IOA that was accepted in the SIAR is 12.44 mg/L at 23.1 °C. The model estimated value (U.S. EPA, 2000c) is very similar, 16.8 mg/L. For

Isodecyl Acrylate, the more hydrophobic ester group, isodecane, will provide for a slightly lower water solubility. The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000c) estimate value for water solubility of Isodecyl Acrylate of 1.75 mg/L is consistent with the expectation of slightly lower solubility than IOA as well as with the known properties of Isodecyl Acrylate. The robustness of the model value for IOA compared to the measured value provides further support for the accuracy of the model estimate of 1.75 mg/L value for Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

6.0 Environmental Fate

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

6.1 Photodegradation

The model prediction for atmospheric photodegradation of Isodecyl Acrylate provides a second order rate of reaction with hydroxyl radicals of $22.2 \text{ E-}12 \text{ cm}^3/\text{molecule-sec}$ and a $t_{1/2}$ of 5.8 hours (U.S. EPA, 2000d). Similar values are estimated for IOA, $19.4 \times 10^{-12} \text{ cm}^3/\text{molecule-sec}$ and 6.6 hours. These data are considered adequate to meet the HPV Program requirements.

6.2 Stability in Water

Esters of acrylate and methacrylate are all hydrolytically stable at acidic and neutral pH. At approximately pH 11, these molecules rapidly (generally with $t_{1/2}$ of minutes) hydrolyze to acrylic acid and the appropriate alcohol. A broad database exists supporting this pH-dependent hydrolysis for these types of molecules, much of which has been submitted in the HPV Chemicals Challenge Program, the OECD SIDS program and others. The pH range relevant to determination of environmental fate is generally between pH 5 and 7. Therefore, hydrolysis is not a significant route of degradation in the environment and additional testing will not further the understanding of the environmental fate of Isodecyl Acrylate. The model is not accurate for determination of hydrolysis but does 'recognize' the hydrolytic stability of the molecule indicating half lives of > 1 year at pH 7 and 8. Based on the extensive background data for acrylic and methacrylic esters, these data are considered adequate to meet the HPV Program requirements.

6.3 Transport and Distribution

Potential environmental exposure to Isodecyl Acrylate is limited based on the use patterns in UV/EB coating applications and the minimal residual monomer levels in final product polymers. Therefore, only accidental releases were considered for the fugacity modeling (U.S. EPA, 2000e). Two scenarios, 100% release to air and 100% release to water were examined. For the air release, the model predicted a distribution of 96% into atmosphere, 1.6% into water, 1% into soil, and 1% into sediment. For the water release, the model predicted a distribution of 1.5% into atmosphere, 60% into water, <0.1% into soil, and 39% into sediment. For completeness, similar estimates were made for IOA (these data were not taken from the accepted SIAR). For the air release of IOA, the model predicted a distribution

of 96% into atmosphere, 3% into water, 1% into soil, and <1% into sediment. For the water release, the model predicted a distribution of 2.4% into atmosphere, 91% into water, <0.1% into soil, and 7% into sediment. These data are considered adequate to meet the HPV Program requirements.

6.4 Biodegradability

As defined in the accepted SIAR, IOA has been shown to be rapidly degraded in an OECD 301D test (72% degradation in 5 days and 100% degradation in 28 days) and is Readily Biodegradable (3M unpublished data). The similar structure of Isodecyl Acrylate indicates that it will also undergo rapid biodegradation in the environment. In addition, the closely related, Isodecyl Methacrylate (submitted in the Hydrophobic Methacrylate Category for ICCA), degraded 88% in 28 days although the 10-day window was not met (Elf Atochem, 2001). These data are considered adequate to meet the HPV Program requirements.

7.0 Ecotoxicity

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

7.1 Toxicity to Fish

The 96-hour LC₅₀ value for the fathead minnow accepted for IOA in the SIAR is 0.67 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to fish. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an LC₅₀ value of 0.9 mg/L for Isodecyl Acrylate consistent with the anticipated toxicity based on the value for IOA. These data are considered adequate to meet the HPV Program requirements.

7.2 Toxicity to Aquatic Invertebrates

The 48-hour EC₅₀ value for *Daphnia magna* accepted for IOA in the SIAR is 0.4 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an EC₅₀ value of 0.55 mg/L for Isodecyl Acrylate consistent with the anticipated toxicity based on the value for IOA. These data are considered adequate to meet the HPV Program requirements.

7.3 Toxicity to Aquatic Plants

The 96-hour EC₅₀ value for algae accepted for IOA in the SIAR is 2.13 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an EC₅₀ value of 0.066 mg/L for Isodecyl Acrylate predicting greater toxicity than expected from the value for IOA. These data are considered adequate to meet the HPV Program requirements.

7.4 Chronic Toxicity to Aquatic Invertebrates

IOA was tested in two reproduction studies with *Daphnia magna* that were accepted as part of the SIAR review. The EC₅₀ values for reproduction in these studies were 1.99 and 1.61 mg/L (3M, unpublished data) confirming that IOA and Isodecyl Acrylate, by analogy, are toxic to aquatic invertebrates. These data are considered adequate to meet the HPV Program requirements.

8.0 Human Health-Related Data

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document. The studies summarized below and in the robust summaries are for IOA.

8.1 Acute Toxicity

The acute oral LD₅₀ in rats for IOA accepted for the SIAR is > 5000 mg/kg body weight (Glaza, 1989; Gordon *et al.*, 1991). This value is consistent with the limited toxicity of hydrophobic acrylate and methacrylate esters and is considered appropriate for Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

8.2 Repeated Dose Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/Developmental Screening Test (Henwood, 1993) that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 1.0%, 7.5%, 15%, or 25% (lowered to 20% after 1 week) IOA in acetone at a dose volume of 100 µL/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4. Dermal irritation, consisting of moderate erythema, slight desquamation, and slight fissuring (females only) was observed in the high dose group. Slight increases in serum aspartate aminotransferase and alanine aminotransferase concentrations were noted in males from the high dose group. No other treatment-related effects were observed. Based on the very limited systemic effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no significant toxicity is anticipated from dermal exposure under current use patterns to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Program requirements.

8.3 Genetic Toxicity

8.3.1 *In vitro*

IOA was tested in a bacterial gene mutation assay according to OECD Guideline 471 with Salmonella strains TA1535, TA1537, TA1538, TA98 and TA100. IOA was negative with and without metabolic activation at concentrations ranging from 0.005 to 0.5 µL/plate (Mortelmans and Pomeroy, 1980; Gordon *et al.*, 1991).

IOA was tested in a mouse lymphoma assay according to OECD Guideline 476. There was no evidence of mutagenicity in this mammalian cell assay at concentrations ranging from 0.0015 to 0.11 µL/plate (Kirby, 1980; Gordon *et al.*, 1991).

Isodecyl Acrylate and IOA are members of a large family of acrylic acid esters. A large battery of mutagenicity screening tests exists for these chemicals and the results of these studies have been submitted in other HPV and ICCA Test Plans. The conclusion that these esters are not mutagenic is consistent for the family as a whole. As concluded in the SIAR for IOA, the exposure and low toxicity of these chemicals indicates that further testing will not provide additional knowledge of the potential hazards. Therefore, consistent with the IOA SIAR, the available data are considered adequate to meet the HPV Program requirements.

8.4 Reproductive and Developmental Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/Developmental Screening Test that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 1.0%, 7.5%, 15%, or 25% (lowered to 20% after 1 week) IOA in acetone at a dose volume of 100 μ L/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4 (see Repeated Dose Toxicity above). There were no treatment-related effects on male fertility, female fertility, mean days to mating, length of gestation, gestation length, pup viability mean number of pups/litter, or pup weights. There were no treatment-related findings at necropsy of the pups. Reproductive organ weight and histopathology findings for the adults were similar to controls. The reproductive and developmental NOAEL was 20%. Based on the lack of effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no reproductive or developmental toxicity is anticipated from exposure under current use patterns to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Program requirements.

9.0 Conclusion

Isodecyl Acrylate and IOA are very similar congeners of a large family of acrylic acid esters. The data for IOA have been used extensively in evaluation of the HPV/SIDS endpoints for Isodecyl Acrylate. Adequate information is available for melting point, boiling point, vapor pressure and partition coefficient for both chemicals. Photodegradation and environmental distributions are adequately supported by the appropriate model data for Isodecyl Acrylate and the model data for IOA support the similarity of the chemicals. Hydrolysis of acrylic acid esters does not occur at physiological or environmental pH. The aquatic tests with fish, invertebrates and plants, for IOA indicates that IOA, Isodecyl Acrylate and other hydrophobic acrylic esters are toxic to aquatic organisms. Since IOA and, therefore, Isodecyl Acrylate, rapidly degrades in the environment and environmental exposure is very limited, the degradation and toxicity studies for IOA are adequate to support Isodecyl Acrylate environmental fate and effects. The LD₅₀ of IOA is >5000 mg/kg and subchronic toxicity evaluations indicate that only skin irritation would be anticipated from exposure to these hydrophobic acrylate esters. IOA is not mutagenic in screening assays consistent with the family of acrylic acid esters. Isodecyl Acrylate, therefore, is also considered not to pose a mutagenic hazard. As with repeated dose studies, evaluation of the reproductive and developmental toxicity of IOA is adequate for Isodecyl Acrylate and indicates that Isodecyl Acrylate does not affect reproduction or the developing offspring. Overall, the available data for IOA, consistent with the conclusions of the SIAM, are considered adequate to meet the HPV Chemical Challenge Program requirements and serve to similarly support Isodecyl Acrylate.

10.0 References

- Elf Atochem. 2001. Determination of Ready Biodegradability CO₂ Evolution Test, Test substance: Isodecyl Methacrylate. Laboratory Study Number 19014 ECS. April 24, 2001. Centre International De Toxicologie (Testing Facility).
- Galloway, S. 2000. Cytotoxicity and Chromosomal Aberrations in vitro: Experience in Industry and the Case for an Upper Limit on Toxicity in the Aberration Assay. *Environmental and Molecular Mutagenesis* 35:191-201.
- Glaza, S. M. 1989. Acute Oral Toxicity Study in Rats (OECD Guidelines). Unpublished report (study no. 81000694), dated February 14, 1989, for Minnesota Mining & Manufacturing Company, St. Paul, MN, USA; by Hazleton Laboratories, Inc., Madison, WI, USA.
- Gordon, S.C., D. D. Zimmerman and F. D. Griffith. 1991. Acute toxicity, genotoxicity and dermal carcinogenicity assessment of IOA. *J. Toxicol. Environ. Health* 34, 279-296.
- Henwood, S. M. 1993. Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Study with 2-Propenoic Acid, Isooctyl Ester (IOA), in Rats via Dermal Application. Unpublished report (no. HWI6329-104), dated March 1, 1993; for 3M Company, St. Paul, MN, USA; by Hazleton Wisconsin, Inc., Madison, WI, USA.
- Howard, P. H. and W. M. Meylan. 1997. *Handbook of Physical Properties of Organic Chemicals*. CRC Press Inc., Lewis Publishers, Boca Raton. p. 578.
- Kirby, P. E. 1980. Evaluation of Test Article T-2476 (MRI#446) for Mutagenic Potential Employing the L5178Y TK[±] Mutagenesis Assay. Unpublished report dated July 17, 1980; for 3M Company, St. Paul, MN, USA; by EG&G Mason Research Institute, Rockville, MD, USA.
- Mortelmans, K. E. and A. Pomeroy. 1980. In vitro Microbiological Assays of 3M Company's Compound T-2476ChR. Unpublished report (SRI Project no. LSC-8958) dated June 1980; for 3M Company, St. Paul, MN, USA; by SRI International, Menlo Park, CA, USA.
- U. S. EPA (U.S. Environmental Protection Agency). 2000a. EPI Suite™, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U. S. EPA (U.S. Environmental Protection Agency). 2000b. EPI Suite™, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

-
- U. S. EPA (U.S. Environmental Protection Agency). 2000c. EPI Suite™, Version 3.11; WSKOW Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000d. EPI Suite™, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000e. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000f. EPI Suite™, Version 3.11; ECOSAR Version 0.99g; PC-Computer software developed by ECOSAR Program, Risk Assessment Division (7403), Washington, D.C.

Table 1: Data Summary				
2-Propenoic Acid, Isodecyl Ester				
CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL PROPERTIES				
2.1	Melting Point		Handbook Data – for Isodecyl Acrylate	-100 °C
2.2	Boiling Point		Handbook Data – for Isodecyl Acrylate	158 °C
2.4	Vapor Pressure		Handbook Data – for Isodecyl Acrylate	0.03 hPa (at 20 °C)
2.5	Partition Coefficient (log K _{ow})		KOWWIN v. 1.67 – for Isodecyl Acrylate	5.07
2.6	Water Solubility		WSKOW v. 1.41 – for Isodecyl Acrylate	1.75 mg/L
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		AOPWIN v. 1.91 – for Isodecyl Acrylate	half-life: 5.8 hours (OH Rate Constant)
3.1.2	Stability in Water			Acrylate esters are stable at pH 3 and 7 and hydrolyze rapidly to acrylate and the associated alkyl chain at pH 11.
3.3	Transport and Distribution		Mackay Level III – for Isodecyl Acrylate 100% release to air	96% into atmosphere, 1.6% into water, 1% into soil, 1% into sediment
			Mackay Level III – for Isodecyl Acrylate 100% release to water	1.5% into atmosphere, 60% into water, <0.1% into soil, 39% into sediment
3.5	Biodegradation		OECD 301D – for IOA	100% after 28 days; Readily Biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish*	<i>Pimephales promelas</i>	OECD 203 – for IOA	LC ₅₀ (96 hours) = 0.67 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD 202 – for IOA	EC ₅₀ (48 hours) = 0.4 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	Green algae	OECD 201 – for IOA	EC ₅₀ (72 hours) = 2.13 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD 202 (2 studies) – for IOA	EC ₅₀ (Reproduction) = 1.99 mg/L EC ₅₀ (Reproduction) = 1.61 mg/L

Table 1: Data Summary				
2-Propenoic Acid, Isodecyl Ester				
CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1	Acute Oral Toxicity	Rat	OECD 401 – for IOA	LD ₅₀ : >5000 mg/kg bw
5.7	Repeated Dose Toxicity	Rat - Dermal	OECD 422 – for IOA	NOAEL = 15% (100 µl/day)
5.8	Genetic Toxicity <i>In Vitro</i> Bacterial Test (Gene mutation)	<i>Salmonella typhimurium</i>	OECD 471 – for IOA	Negative
		Mouse lymphoma	OECD 476 – for IOA	Negative
5.11	Toxicity to Reproduction / Impairment of Fertility	Rat - Dermal	OECD 422 – for IOA	NOAEL > 20% (100 µl/day)
5.12	Developmental Toxicity / Teratogenicity	Rat - Dermal	OECD 422 – for IOA	NOAEL > 20% (100 µl/day)