

Biodegradation

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E423

201-15047B

PROPYLENE STREAMS ROBUST SUMMARY

Biodegradation

RECEIVED
 OPERATIONS
 01 JAN 14 PM 1:42

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Inoculum:	Not applicable
Exposure Period:	Not applicable
Test Conditions:	Not applicable
<ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	
Results:	Not applicable
Units/Value:	
<ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	
Test Substance:	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p>

Conclusion:	<p><u>Summary</u></p> <p>In the environment, biodegradation will not contribute significantly to the loss of chemicals in substances from the Propylene Streams Category. The Propylene Streams Category includes four process streams:</p> <ul style="list-style-type: none">• Propylene, polymer grade• Propylene, chemical grade• Propylene Stream• Light Ends from Butadiene Plant <p>Two CAS numbers (see <u>Test Substance</u>) identify substances derived from these process streams. The substances contain various chemicals composed of carbon and hydrogen. As discussed below, substances in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that substances from this category will partition to environmental compartments where they could be degraded by bacteria.</p> <p><u>The Propylene Streams Category</u></p> <p>A process stream is a mixture of substances that arises from a chemical reaction or separation activity. The process streams in this category include two propylene grades and two propylene-containing streams. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C2-C3. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Propylene Streams</u>.</p> <p>The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).</p> <p>Propylene streams arise from production processes associated with ethylene manufacturing. More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the four process streams in this category are:</p> <ul style="list-style-type: none">• Propylene, polymer grade is a high purity (99%+) product of the ethylene unit. It is obtained by fractionation of a portion of the condensed cracking furnace effluent and other processing
--------------------	---

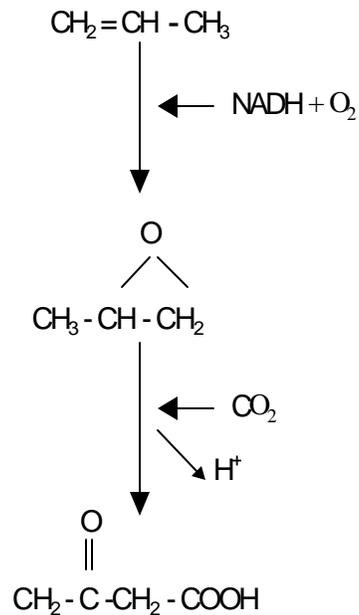
	<p>steps (e.g. C3 acetylene removal). The final polymer grade propylene is produced as the distillate from the C3 splitter. The main impurities of the stream are typically ethane and propane.</p> <ul style="list-style-type: none">• Propylene, chemical grade is a C3 product with typical propylene content of 93 to 95%. Propane accounts for most of the balance of the composition. An ethylene process using a scheme similar to that used for polymer grade propylene, but with fewer or less rigorous purification steps, produces this grade.• Propylene Stream is the C3 stream prior to separation into propylene and propane. Typically, this stream is produced as the overhead from the depropanizer in an ethylene unit. It is a narrow boiling-range mixture that consists predominantly of C3 hydrocarbons. A typical composition is 85% propylene, 12% propane, and 3% C3 acetylenes.• Light Ends from Butadiene Plant is produced by fractionation of the C4 Crude Butadiene to remove relatively low levels of propane and propylene that may be contained in the stream. The carbon number distribution for the stream is predominantly C3. <p><u>Biodegradation of Hydrocarbons</u></p> <p>Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.</p> <p>Substances in the Propylene Streams Category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C3. Consequently, their availability to microbial degraders will be significantly limited.</p> <p>Component substances from all four process streams in this category are simple hydrocarbons, which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical attack) for specific degradation rates of selected substances from this category; AOP data were developed for this category under the HPV Chemical Program]. All substances from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of substances in this category, biodegradative processes will be less likely to contribute to their loss from the environment.</p> <p>Substances from the Propylene Streams Category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for substances in this</p>
--	--

category that demonstrates that they can be biodegraded.

Watkinson and Morgan (6) state that microbial metabolism of aliphatic alkenes, such as those in the Propylene Streams Category, can be initiated by attack at the double bond. Four degradative processes have been identified:

- oxygenase attack upon a terminal methyl group to the corresponding unsaturated alcohol and acid,
- subterminal oxygenase attack to the corresponding alcohol and acid,
- oxidation across the double bond to the corresponding epoxide, and
- oxidation across the double bond to the corresponding diol.

Experimental studies to determine a catabolic pathway for propylene as mediated by a *Xanthobacter* sp. (3) resulted in the following proposed series of reactions:



The degradation of propylene leads to acetoacetate which is the entry compound into intermediary metabolism.

The potential biodegradability of some of the other components including ethylene and propane has been summarized and metabolic pathways leading to their biodegradation have been described (4, 5). These compounds have been shown to biodegrade to high extents such that if they were to partition to

Biodegradation

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E423

	<p>either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment.</p> <p>In summary, because the C3 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Overall, products from this category and their component chemicals are expected to degrade rapidly in the environment and not persist.</p> <p>References</p> <ol style="list-style-type: none">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA.2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA.3. Small, F.J. and S.A. Ensign. 1995. Carbon Dioxide Fixation in the Metabolism of Propylene and Propylene Oxide by <i>Xanthobacter</i> Strain Py2. <i>Journal of Bacteriology</i>. Vol. 177 (21) pp. 6170-6175.4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA.5. Hartmans, S. 1993. Biodegradation of chlorinated and unsaturated hydrocarbons in relation to biological waste-gas treatment. Thesis Wageningen University. NL.6. Watkinson, R.J. and P. Morgan. 1990. Physiology of aliphatic hydrocarbon-degrading microorganisms. <i>Biodegradation</i>. 1:79-92.
Reliability:	These data represent a key study for characterizing the potential of substances in the Propylene Streams Category to undergo biodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Biodegradation: Propylene Streams Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "biodegradation". Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Boiling Point (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E460

PROPYLENE STREAMS ROBUST SUMMARY**Boiling Point**

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: <ul style="list-style-type: none">Note: Concentration prep., vessel type, replication, test conditions.	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: Units/Value: <ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	<p>Calculated and measured boiling point data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential boiling point range for substances represented by the two CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the boiling point range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p>

Boiling Point (Range)**CAS No.:** 115-07-1; 68606-26-8**Robust Summary No.:** OP E460

Results: (continued) Units/Value: Note: Deviations from protocol or guideline, analytical method.	<table border="1"><thead><tr><th data-bbox="690 289 836 352"><u>Substance Constituent</u></th><th data-bbox="938 289 1068 352"><u>Calculated BP (°C)</u></th><th data-bbox="1177 289 1307 352"><u>Measured* BP (°C)</u></th></tr></thead><tbody><tr><td data-bbox="690 384 836 415">propadiene</td><td data-bbox="966 384 1040 415">-18.32</td><td data-bbox="1205 384 1279 415">-34.4</td></tr><tr><td data-bbox="690 415 836 447">propylene</td><td data-bbox="977 415 1040 447">-9.84</td><td data-bbox="1205 415 1279 447">-47.6</td></tr><tr><td data-bbox="690 447 836 478">propane</td><td data-bbox="977 447 1040 478">-7.76</td><td data-bbox="1205 447 1279 478">-42.1</td></tr></tbody></table> <p data-bbox="690 506 1458 596">* Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>	propadiene	-18.32	-34.4	propylene	-9.84	-47.6	propane	-7.76	-42.1
<u>Substance Constituent</u>	<u>Calculated BP (°C)</u>	<u>Measured* BP (°C)</u>											
propadiene	-18.32	-34.4											
propylene	-9.84	-47.6											
propane	-7.76	-42.1											
Test Substance:	<p data-bbox="690 640 1409 703">The Propylene Streams Category includes the following CAS numbers:</p> <table border="0" data-bbox="690 720 1076 783"><tr><td data-bbox="690 720 803 751">115-07-1</td><td data-bbox="857 720 982 751">1-Propene</td></tr><tr><td data-bbox="690 751 836 783">68606-26-8</td><td data-bbox="857 751 1076 783">Hydrocarbons, C3</td></tr></table> <p data-bbox="690 814 1469 993">Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p data-bbox="690 1024 1453 1119">More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol data-bbox="690 1150 1469 1297" style="list-style-type: none"><li data-bbox="690 1150 1469 1297">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.	115-07-1	1-Propene	68606-26-8	Hydrocarbons, C3								
115-07-1	1-Propene												
68606-26-8	Hydrocarbons, C3												
Conclusion:	<p data-bbox="690 1312 1469 1444">Based on calculated constituent data, substances in this category can have a boiling range of -7.76 to -18.32°C @ 760 mm Hg. Based on measured constituent data, substances in this category can have a boiling range of -34.4 to -47.6°C @ 760 mm Hg.</p>												
Reliability:	<p data-bbox="690 1470 1019 1501">(2) Reliable with restrictions</p> <p data-bbox="690 1533 1477 1864">The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.</p>												

Boiling Point (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E460

Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Calculated Alga Toxicity

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E448

PROPYLENE STREAMS ROBUST SUMMARY

Alga Toxicity

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]												
Method/Guideline*:	Other: ECOSAR Computer Model												
Year (guideline):	1999												
Type (test type):	Green Alga Toxicity Calculation; EC50												
GLP:	Not applicable												
Year (study performed):	Not applicable												
Species:	Freshwater Green Alga (calculated toxicity values are not species specific)												
Analytical Monitoring:	Not applicable												
Exposure Period:	96 hours												
Statistical Method:*	Not applicable												
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN, a subroutine in the EPIWIN computer model (1), which is based on an atom/fragment contribution method of Meylan and Howard (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Propylene Streams Category, are listed below.</p> <table border="1"> <thead> <tr> <th><u>Substance Constituent</u></th> <th><u>Calculated log K_{ow}</u></th> <th><u>Measured* log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td>1.67</td> <td>1.45</td> </tr> <tr> <td>propylene</td> <td>1.68</td> <td>1.77</td> </tr> <tr> <td>propane</td> <td>1.81</td> <td>2.36</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <ol style="list-style-type: none"> Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 	<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Measured* log K_{ow}</u>	propadiene	1.67	1.45	propylene	1.68	1.77	propane	1.81	2.36
<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Measured* log K_{ow}</u>											
propadiene	1.67	1.45											
propylene	1.68	1.77											
propane	1.81	2.36											

Calculated Alga Toxicity

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E448

<p>Results:</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method, biological observations, control survival. 	<p>Calculated alga toxicity values for three chemicals representative of substances in the Propylene Streams Category are listed below.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the acute toxicity range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p> <table border="0"> <thead> <tr> <th style="text-align: left;"><u>Substance Constituent</u></th> <th style="text-align: center;"><u>Calculated log K_{ow}</u></th> <th style="text-align: center;"><u>Alga Toxicity 96-hr EC50 (mg/L)</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">1.67</td> <td style="text-align: center;">40.6</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">1.68</td> <td style="text-align: center;">40.1</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">1.81</td> <td style="text-align: center;">32.3</td> </tr> </tbody> </table> <table border="0"> <thead> <tr> <th style="text-align: left;"><u>Substance Constituent</u></th> <th style="text-align: center;"><u>Measured* log K_{ow}</u></th> <th style="text-align: center;"><u>Alga Toxicity 96-hr EC50 (mg/L)</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">1.45</td> <td style="text-align: center;">61.0</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">1.77</td> <td style="text-align: center;">33.4</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">2.36</td> <td style="text-align: center;">10.5</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <p>The data represent a potential acute toxicity range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Alga Toxicity 96-hr EC50 (mg/L)</u>	propadiene	1.67	40.6	propylene	1.68	40.1	propane	1.81	32.3	<u>Substance Constituent</u>	<u>Measured* log K_{ow}</u>	<u>Alga Toxicity 96-hr EC50 (mg/L)</u>	propadiene	1.45	61.0	propylene	1.77	33.4	propane	2.36	10.5
<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Alga Toxicity 96-hr EC50 (mg/L)</u>																							
propadiene	1.67	40.6																							
propylene	1.68	40.1																							
propane	1.81	32.3																							
<u>Substance Constituent</u>	<u>Measured* log K_{ow}</u>	<u>Alga Toxicity 96-hr EC50 (mg/L)</u>																							
propadiene	1.45	61.0																							
propylene	1.77	33.4																							
propane	2.36	10.5																							
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial substances or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3. The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures and if released to the environment are expected to partition largely to the air.</p>																								

Calculated Alga Toxicity

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E448

	<p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures.</p> <p>Based on calculated K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 32.3 to 40.6 mg/L. Based on measured K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 10.5 to 61.0 mg/L.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic plants based on constituent data.</p>
Reference:	<p>Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.</p>
Other (source):	<p>American Chemistry Council, Olefins Panel (Prepared 1/03)</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to aquatic plants". Selecting this option refers the reader to information in the "freetext" field for "test substance".

PROPYLENE STREAMS ROBUST SUMMARY

Fish Acute Toxicity

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]												
Method/Guideline*:	Other: ECOSAR Computer Model												
Year (guideline):	1999												
Type (test type):	Acute Fish Toxicity Calculation; LC50												
GLP:	Not applicable												
Year (study performed):	Not applicable												
Species:	Freshwater Fish (calculated toxicity values are not species specific)												
Analytical Monitoring:	Not applicable												
Exposure Period:	96 hours												
Statistical Method:	Not applicable												
Test Conditions: <ul style="list-style-type: none"> • Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN, a subroutine in the EPIWIN computer model (1), which is based on an atom/fragment contribution method of Meylan and Howard (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Propylene Streams Category, are listed below.</p> <table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>Substance Constituent</u></th> <th style="text-align: center;"><u>Calculated log K_{ow}</u></th> <th style="text-align: center;"><u>Measured* log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">1.67</td> <td style="text-align: center;">1.45</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">1.68</td> <td style="text-align: center;">1.77</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">1.81</td> <td style="text-align: center;">2.36</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <ol style="list-style-type: none"> 1. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. 2. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 	<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Measured* log K_{ow}</u>	propadiene	1.67	1.45	propylene	1.68	1.77	propane	1.81	2.36
<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Measured* log K_{ow}</u>											
propadiene	1.67	1.45											
propylene	1.68	1.77											
propane	1.81	2.36											

Calculated Fish Acute Toxicity

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E450

<p>Results:</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method, biological observations, control survival. 	<p>Calculated fish acute toxicity values for three chemicals representative of substances in the Propylene Streams Category are listed below.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the acute toxicity range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p> <table border="0"> <thead> <tr> <th style="text-align: left;"><u>Substance</u> <u>Constituent</u></th> <th style="text-align: center;">Calculated <u>log K_{ow}</u></th> <th style="text-align: center;">Fish Acute <u>96-hr LC50 (mg/L)</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">1.67</td> <td style="text-align: center;">63.4</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">1.68</td> <td style="text-align: center;">62.4</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">1.81</td> <td style="text-align: center;">49.3</td> </tr> </tbody> </table> <table border="0"> <thead> <tr> <th style="text-align: left;"><u>Substance</u> <u>Constituent</u></th> <th style="text-align: center;">Measured* <u>log K_{ow}</u></th> <th style="text-align: center;">Fish Acute <u>96-hr LC50 (mg/L)</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">1.45</td> <td style="text-align: center;">97.7</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">1.77</td> <td style="text-align: center;">51.3</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">2.36</td> <td style="text-align: center;">15.0</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <p>The data represent a potential acute toxicity range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	<u>Substance</u> <u>Constituent</u>	Calculated <u>log K_{ow}</u>	Fish Acute <u>96-hr LC50 (mg/L)</u>	propadiene	1.67	63.4	propylene	1.68	62.4	propane	1.81	49.3	<u>Substance</u> <u>Constituent</u>	Measured* <u>log K_{ow}</u>	Fish Acute <u>96-hr LC50 (mg/L)</u>	propadiene	1.45	97.7	propylene	1.77	51.3	propane	2.36	15.0
<u>Substance</u> <u>Constituent</u>	Calculated <u>log K_{ow}</u>	Fish Acute <u>96-hr LC50 (mg/L)</u>																							
propadiene	1.67	63.4																							
propylene	1.68	62.4																							
propane	1.81	49.3																							
<u>Substance</u> <u>Constituent</u>	Measured* <u>log K_{ow}</u>	Fish Acute <u>96-hr LC50 (mg/L)</u>																							
propadiene	1.45	97.7																							
propylene	1.77	51.3																							
propane	2.36	15.0																							
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial substances or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3. The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures and if released to the environment are expected to partition largely to the air.</p>																								

Calculated Fish Acute Toxicity

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E450

	<p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures.</p> <p>Based on calculated K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 49.3 to 63.4 mg/L. Based on measured K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 15.0 to 97.7 mg/L.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to fish based on constituent data.</p>
Reference:	<p>Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.</p>
Other (source):	<p>American Chemistry Council, Olefins Panel (P repared 1/03)</p>

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to fish". Selecting this option refers the reader to information in the "freetext" field for "test substance".

PROPYLENE STREAMS ROBUST SUMMARY

Daphnid Acute Toxicity

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]												
Method/Guideline*:	Other: ECOSAR Computer Model												
Year (guideline):	1999												
Type (test type):	Acute Daphnid Toxicity Calculation; LC50												
GLP:	Not applicable												
Year (study performed):	Not applicable												
Species:	Daphnid (calculated toxicity values are not species specific)												
Analytical Monitoring:	Not applicable												
Exposure Period:	48 hours												
Statistical Method:	Not applicable												
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 	<p>Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN, a subroutine in the EPIWIN computer model (1), which is based on an atom/fragment contribution method of Meylan and Howard (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Propylene Streams Category, are listed below.</p> <table border="1"> <thead> <tr> <th>Substance <u>Constituent</u></th> <th>Calculated <u>log K_{ow}</u></th> <th>Measured* <u>log K_{ow}</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td>1.67</td> <td>1.45</td> </tr> <tr> <td>propylene</td> <td>1.68</td> <td>1.77</td> </tr> <tr> <td>propane</td> <td>1.81</td> <td>2.36</td> </tr> </tbody> </table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <ol style="list-style-type: none"> Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 	Substance <u>Constituent</u>	Calculated <u>log K_{ow}</u>	Measured* <u>log K_{ow}</u>	propadiene	1.67	1.45	propylene	1.68	1.77	propane	1.81	2.36
Substance <u>Constituent</u>	Calculated <u>log K_{ow}</u>	Measured* <u>log K_{ow}</u>											
propadiene	1.67	1.45											
propylene	1.68	1.77											
propane	1.81	2.36											

Calculated Daphnid Acute Toxicity

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E449

<p>Results:</p> <p>Units/Value:</p> <ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<p>Calculated daphnid acute toxicity values for three chemicals representative of substances in the Propylene Streams Category are listed below.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the acute toxicity range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p> <table border="1"><thead><tr><th><u>Substance Constituent</u></th><th><u>Calculated log K_{ow}</u></th><th><u>Daphnid Acute 48-hr LC50 (mg/L)</u></th></tr></thead><tbody><tr><td>propadiene</td><td>1.67</td><td>66.3</td></tr><tr><td>propylene</td><td>1.68</td><td>65.4</td></tr><tr><td>propane</td><td>1.81</td><td>52.2</td></tr></tbody></table> <table border="1"><thead><tr><th><u>Substance Constituent</u></th><th><u>Measured* log K_{ow}</u></th><th><u>Daphnid Acute 48-hr LC50 (mg/L)</u></th></tr></thead><tbody><tr><td>propadiene</td><td>1.45</td><td>100.8</td></tr><tr><td>propylene</td><td>1.77</td><td>54.1</td></tr><tr><td>propane</td><td>2.36</td><td>16.5</td></tr></tbody></table> <p>* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.</p> <p>The data represent a potential acute toxicity range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Daphnid Acute 48-hr LC50 (mg/L)</u>	propadiene	1.67	66.3	propylene	1.68	65.4	propane	1.81	52.2	<u>Substance Constituent</u>	<u>Measured* log K_{ow}</u>	<u>Daphnid Acute 48-hr LC50 (mg/L)</u>	propadiene	1.45	100.8	propylene	1.77	54.1	propane	2.36	16.5
<u>Substance Constituent</u>	<u>Calculated log K_{ow}</u>	<u>Daphnid Acute 48-hr LC50 (mg/L)</u>																							
propadiene	1.67	66.3																							
propylene	1.68	65.4																							
propane	1.81	52.2																							
<u>Substance Constituent</u>	<u>Measured* log K_{ow}</u>	<u>Daphnid Acute 48-hr LC50 (mg/L)</u>																							
propadiene	1.45	100.8																							
propylene	1.77	54.1																							
propane	2.36	16.5																							

Calculated Daphnid Acute Toxicity

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E449

Test Substance:	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3. The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures and if released to the environment are expected to partition largely to the air.</p> <p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>The substances in the Propylene Streams Category are gaseous at environmentally relevant temperatures.</p> <p>Based on calculated K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 52.2 to 66.3 mg/L. Based on measured K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 16.5 to 100.8 mg/L.</p>
Reliability:	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic invertebrates based on constituent data.</p>

Calculated Daphnid Acute Toxicity

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E449

Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to aquatic invertebrates". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Photodegradation (Direct)

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E468

PROPYLENE STREAMS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: <ul style="list-style-type: none"> • Wave length value (upper/lower) 	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: <ul style="list-style-type: none"> • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol 	Not applicable
Direct Photolysis**: <ul style="list-style-type: none"> • Results: half-life, % degradation, quantum yield 	<p><u>Summary</u></p> <p>In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Propylene Streams Category. The Propylene Streams Category includes four process streams:</p> <ul style="list-style-type: none"> • Propylene, polymer grade • Propylene, chemical grade • Propylene Stream • Light Ends from Butadiene Plant <p>Two CAS numbers (see <u>Test Substance</u>) identify substances derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis.</p>

	<p><u>The Propylene Streams Category</u></p> <p>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category include two propylene grades and two propylene-containing streams. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C2-C3. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Propylene Streams</u>.</p> <p>The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).</p> <p>Propylene streams arise from production processes associated with ethylene manufacturing. More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the four process streams in this category are:</p> <ul style="list-style-type: none">• Propylene, polymer grade is a high purity (99%+) product of the ethylene unit. It is obtained by fractionation of a portion of the condensed cracking furnace effluent and other processing steps (e.g. C3 acetylene removal). The final polymer grade propylene is produced as the distillate from the C3 splitter. The main impurities of the stream are typically ethane and propane.• Propylene, chemical grade is a C3 product with typical propylene content of 93 to 95%. Propane accounts for most of the balance of the composition. An ethylene process using a scheme similar to that used for polymer grade propylene, but with fewer or less rigorous purification steps, produces this grade.• Propylene Stream is the C3 stream prior to separation into propylene and propane. Typically, this stream is produced as the overhead from the depropanizer in an ethylene unit. It is a narrow boiling-range mixture that consists predominantly of C3 hydrocarbons. A typical composition is 85% propylene, 12% propane, and 3% C3 acetylenes.• Light Ends from Butadiene Plant is produced by fractionation of the C4 Crude Butadiene to remove relatively low levels of propane and propylene that may be contained in the stream. The carbon number distribution for the stream is predominantly C3.
--	---

Photolysis of Hydrocarbons

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ϵ) for selected unsaturated hydrocarbons are shown below (2):

<u>Hydrocarbon</u>	<u>l below 290 nm</u>		<u>l above 290 nm</u>	
	<u>λ_{max}</u>	<u>ϵ</u>	<u>λ_{max}</u>	<u>ϵ</u>
Ethylene	193	10,000	-	-
1,3-Butadiene	217	2,090	-	-
Benzene	255	215	-	-

Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Propylene Streams category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).

Substances in the Propylene Streams Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

Photodegradation (Direct)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E468

<p>Direct Photolysis**: (continued)</p> <p>Results: half-life, % degradation, quantum yield</p>	<p>References</p> <ol style="list-style-type: none"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
<p>Indirect Photolysis**:</p> <ul style="list-style-type: none"> • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life 	<p>Not applicable</p>
<p>Degradation Products**:</p> <ul style="list-style-type: none"> • Note: Identification, concentration 	<p>Unknown</p>
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p>
<p>Conclusion:</p>	<p>Not applicable</p>
<p>Reliability:</p>	<p>These data represent a key study for characterizing the potential of substances in the Propylene Streams Category to undergo direct photodegradation.</p>
<p>Reference:</p>	<p>American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): Propylene Streams Category. Rosslyn, VA, USA.</p>
<p>Other (source):</p>	<p>American Chemistry Council, Olefins Panel (Prepared 1/03)</p>

* **Other TS** is a selection option under the **Test Substance** pick list that is in the IUCLID entry field for **Photodegradation (Direct)**. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Photodegradation (Indirect)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E470

PROPYLENE STREAMS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: <ul style="list-style-type: none">• Wave length value (upper/lower)	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: <ul style="list-style-type: none">• Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E ⁶ OH radicals/cm ³
Direct Photolysis**: Results: half-life, % degradation, quantum yield	Not applicable

<p>Indirect Photolysis**:</p> <ul style="list-style-type: none"> • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life 	<p><u>The Propylene Streams Category</u></p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Propylene Streams</u>.</p> <p>The three chemicals selected to represent the atmospheric oxidation potential of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p> <p><u>Atmospheric Oxidation of Hydrocarbons</u></p> <p>In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).</p> <p>AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.</p> <p>Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.</p> <table style="margin-left: auto; margin-right: auto; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; border-bottom: 1px solid black;"><u>Chemical</u></th> <th style="text-align: center; border-bottom: 1px solid black;"><u>Calculated* half-life (hrs)</u></th> <th style="text-align: center; border-bottom: 1px solid black;"><u>OH- Rate Constant (cm³/molecule-sec)</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">13.1</td> <td style="text-align: center;">9.8 E⁻¹²</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">4.9</td> <td style="text-align: center;">26.4 E⁻¹²</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">101.2</td> <td style="text-align: center;">1.3 E⁻¹²</td> </tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p>	<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>	propadiene	13.1	9.8 E ⁻¹²	propylene	4.9	26.4 E ⁻¹²	propane	101.2	1.3 E ⁻¹²
<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>											
propadiene	13.1	9.8 E ⁻¹²											
propylene	4.9	26.4 E ⁻¹²											
propane	101.2	1.3 E ⁻¹²											

Photodegradation (Indirect)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E470

<p>Indirect Photolysis**: (cont'd)</p> <p>Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</p>	<p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).</p> <p><u>References:</u></p> <ol style="list-style-type: none"> 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. <i>Environ. Toxicol. Chem.</i> 7:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. <i>Chemosphere</i> 12:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
<p>Degradation Products**:</p> <ul style="list-style-type: none"> • Note: Identification, concentration 	<p>Unknown</p>
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p>
<p>Conclusion:</p>	<p>Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 4.9 to 101.2 hours as a result of indirect photolysis by hydroxyl radical attack.</p>
<p>Reliability:</p>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 2 CAS numbers under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.</p>

Photodegradation (Indirect)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E470

Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

** In IUCLID, provide additional discussion if needed in the results freetext

Hydrolysis (Stability in Water)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E467

PROPYLENE STREAMS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: <ul style="list-style-type: none">• Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol	Not applicable
Results: Units/Value: <ul style="list-style-type: none">• Note: Analytical method, observations, half-lives by pH, degradation products	Not applicable
Test Substance:	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>

<p>Conclusion:</p>	<p><u>Summary</u></p> <p>In the environment, hydrolysis will not contribute to the degradation of substances in the Propylene Streams Category. The Propylene Streams category includes four process streams:</p> <ul style="list-style-type: none">• Propylene, polymer grade• Propylene, chemical grade• Propylene Stream• Light Ends from Butadiene Plant <p>Two CAS numbers (see <u>Test Substance</u>) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.</p> <p><u>The Propylene Streams Category</u></p> <p>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category include two propylene grades and two propylene-containing streams. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C2-C3. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Propylene Streams</u>.</p> <p>The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).</p> <p>Propylene streams arise from production processes associated with ethylene manufacturing. More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the four process streams in this category are:</p> <ul style="list-style-type: none">• Propylene, polymer grade is a high purity (99%+) product of the ethylene unit. It is obtained by fractionation of a portion of the condensed cracking furnace effluent and other processing steps (e.g. C3 acetylene removal). The final polymer grade propylene is produced as the distillate from the C3 splitter. The main impurities of the stream are typically ethane and propane.• Propylene, chemical grade is a C3 product with typical propylene content of 93 to 95%. Propane accounts for most of the balance of the composition. An ethylene process using a scheme similar to that used for polymer grade propylene, but with fewer or less rigorous purification steps, produces this grade.
---------------------------	---

	<ul style="list-style-type: none">• Propylene Stream is the C3 stream prior to separation into propylene and propane. Typically, this stream is produced as the overhead from the depropanizer in an ethylene unit. It is a narrow boiling-range mixture that consists predominantly of C3 hydrocarbons. A typical composition is 85% propylene, 12% propane, and 3% C3 acetylenes.• Light Ends from Butadiene Plant is produced by fractionation of the C4 Crude Butadiene to remove relatively low levels of propane and propylene that may be contained in the stream. The carbon number distribution for the stream is predominantly C3. <p><u>Hydrolysis of Hydrocarbons as a Function of Molecular Structure</u></p> <p>Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H₂O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.</p> <p>The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.</p> <p>Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Propylene Streams category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).</p> <p>The substances in the Propylene Streams category are primarily olefins that contain at least one double bond (alkenes). The remaining substances are saturated hydrocarbons (alkanes). These two groups of substances contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, substances in the Propylene Streams Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.</p> <p><u>References</u></p> <ol style="list-style-type: none">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
--	--

Hydrolysis (Stability in Water)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E467

	<ol style="list-style-type: none">2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the Propylene Streams Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis: Propylene Streams Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Partition Coefficient (Range)

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E463

PROPYLENE STREAMS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<p>Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. <i>J. Pharm. Sci.</i> 84: 83-92.</p>
Results: Units/Value: <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated and measured log K_{ow} data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential log K_{ow} range for substances represented by the two CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the log K_{ow} range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p>

Partition Coefficient (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E463

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th>Substance Constituent</th> <th>Calculated log K_{ow} @ 25°C</th> <th>Measured* log K_{ow} @ 25°C</th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td>1.65</td> <td>1.45</td> </tr> <tr> <td>propylene</td> <td>1.68</td> <td>1.77</td> </tr> <tr> <td>propane</td> <td>1.81</td> <td>2.36</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C	propadiene	1.65	1.45	propylene	1.68	1.77	propane	1.81	2.36
Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C											
propadiene	1.65	1.45											
propylene	1.68	1.77											
propane	1.81	2.36											
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 												
<p>Conclusion:</p>	<p>Based on calculated constituent data, substances in this category can have a log K_{ow} range of 1.65 to 1.81 @ 25°C. Based on measured constituent data, substances in this category can have a log K_{ow} range of 1.45 to 2.36 @ 25°C.</p>												
<p>Reliability:</p>	<p>(2) Reliable with restrictions</p> <p>The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.</p>												

Partition Coefficient (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E463

Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Melting Point (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E461

PROPYLENE STREAMS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: <ul style="list-style-type: none">Note: Concentration prep., vessel type, replication, test conditions.	<p>Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle.</p> <p>Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In <u>The Properties of Gases and Liquids</u>. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.</p> <p>The Gold and Ogle Method simply uses the formula $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin.</p>
Results: Units/Value: <ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	<p>Calculated and measured melting point data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential melting point range for substances represented by the two CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the melting point range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p>

Melting Point (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E461

Results: (continued) Units/Value: Note: Deviations from protocol or guideline, analytical method.	<table border="1"><thead><tr><th data-bbox="690 289 836 352"><u>Substance Constituent</u></th><th data-bbox="938 289 1068 352"><u>Calculated MP (°C)</u></th><th data-bbox="1177 289 1307 352"><u>Measured* MP (°C)</u></th></tr></thead><tbody><tr><td data-bbox="690 384 836 411">propadiene</td><td data-bbox="946 384 1027 411">-132.9</td><td data-bbox="1185 384 1266 411">-136.2</td></tr><tr><td data-bbox="690 415 836 443">propylene</td><td data-bbox="946 415 1027 443">-135.4</td><td data-bbox="1185 415 1266 443">-185.2</td></tr><tr><td data-bbox="690 447 836 474">propane</td><td data-bbox="946 447 1027 474">-133.9</td><td data-bbox="1185 447 1266 474">-187.6</td></tr></tbody></table> <p data-bbox="690 506 1469 600">* Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated MP (°C)</u>	<u>Measured* MP (°C)</u>	propadiene	-132.9	-136.2	propylene	-135.4	-185.2	propane	-133.9	-187.6
<u>Substance Constituent</u>	<u>Calculated MP (°C)</u>	<u>Measured* MP (°C)</u>											
propadiene	-132.9	-136.2											
propylene	-135.4	-185.2											
propane	-133.9	-187.6											
Test Substance:	<p data-bbox="690 642 1412 705">The Propylene Streams Category includes the following CAS numbers:</p> <table border="0" data-bbox="690 720 1079 783"><tr><td data-bbox="690 720 803 747">115-07-1</td><td data-bbox="852 720 982 747">1-Propene</td></tr><tr><td data-bbox="690 751 836 779">68606-26-8</td><td data-bbox="852 751 1079 779">Hydrocarbons, C3</td></tr></table> <p data-bbox="690 814 1469 993">Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p data-bbox="690 1024 1453 1119">More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol data-bbox="690 1150 1469 1297" style="list-style-type: none"><li data-bbox="690 1150 1469 1297">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.	115-07-1	1-Propene	68606-26-8	Hydrocarbons, C3								
115-07-1	1-Propene												
68606-26-8	Hydrocarbons, C3												
Conclusion:	<p data-bbox="690 1314 1469 1440">Based on calculated constituent data, substances in this category can have a melting range of -132.9 to -135.4 °C. Based on measured constituent data, substances in this category can have a melting range of -136.2 to -187.6 °C.</p>												
Reliability:	<p data-bbox="690 1482 1015 1514">(2) Reliable with restrictions</p> <p data-bbox="690 1545 1477 1881">The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.</p>												

Melting Point (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E461

Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

PROPYLENE STREAMS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	<p>The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.</p> <p>Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).</p> <p>1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.</p>

<p>Results:</p> <p>Units/Value:</p> <ul style="list-style-type: none"> • Note: Deviations from protocol or guideline, analytical method. 	<p>Calculated partitioning data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential distribution for substances represented by the two CAS numbers under <u>Test Substance</u>. Actual distribution of substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the environmental distribution range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p> <p>The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.</p> <p>The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:</p> <table border="1" style="margin-left: auto; margin-right: auto; border-collapse: collapse;"> <thead> <tr> <th rowspan="3" style="text-align: left; vertical-align: bottom;"><u>Substance Constituent</u></th> <th colspan="2" style="text-align: center;"><u>Calculated*</u></th> <th colspan="2" style="text-align: center;"><u>Measured**</u></th> </tr> <tr> <th colspan="2" style="text-align: center;"><u>Percent Distribution</u></th> <th colspan="2" style="text-align: center;"><u>Percent Distribution</u></th> </tr> <tr> <th style="text-align: center;"><u>Air</u></th> <th style="text-align: center;"><u>Water</u></th> <th style="text-align: center;"><u>Air</u></th> <th style="text-align: center;"><u>Water</u></th> </tr> </thead> <tbody> <tr> <td>propadiene</td> <td style="text-align: center;">99.97</td> <td style="text-align: center;">0.03</td> <td style="text-align: center;">99.96</td> <td style="text-align: center;">0.04</td> </tr> <tr> <td>propylene</td> <td style="text-align: center;">99.98</td> <td style="text-align: center;">0.02</td> <td style="text-align: center;">99.99</td> <td style="text-align: center;">0.01</td> </tr> <tr> <td>propane</td> <td style="text-align: center;">98.44</td> <td style="text-align: center;">1.47</td> <td style="text-align: center;">99.47</td> <td style="text-align: center;">0.43</td> </tr> </tbody> </table> <p>* Distribution values determined using calculated input data from EPIWIN program ** Distribution values determined using input data from the EPIWIN program experimental database</p> <p>The remaining percentage (0.06 to 0.09%) of propane was calculated to partition to the soil. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals.</p>	<u>Substance Constituent</u>	<u>Calculated*</u>		<u>Measured**</u>		<u>Percent Distribution</u>		<u>Percent Distribution</u>		<u>Air</u>	<u>Water</u>	<u>Air</u>	<u>Water</u>	propadiene	99.97	0.03	99.96	0.04	propylene	99.98	0.02	99.99	0.01	propane	98.44	1.47	99.47	0.43
<u>Substance Constituent</u>	<u>Calculated*</u>		<u>Measured**</u>																										
	<u>Percent Distribution</u>		<u>Percent Distribution</u>																										
	<u>Air</u>	<u>Water</u>	<u>Air</u>	<u>Water</u>																									
propadiene	99.97	0.03	99.96	0.04																									
propylene	99.98	0.02	99.99	0.01																									
propane	98.44	1.47	99.47	0.43																									

<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"> 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
<p>Conclusion:</p>	<p>The partitioning data represent a potential distribution range for substances in the two CAS numbers listed under <u>Test Substance</u>. Substances in the Propylene Streams Category are calculated to partition primarily to air with a smaller percentage partitioning to water. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.</p> <p>The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.</p>
<p>Reliability:</p>	<p>(2) Reliable with restrictions</p> <p>The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the two CAS numbers listed under <u>Test Substance</u>. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.</p>

Transport / Distribution (Fugacity)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E469

Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Vapor Pressure (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E462

PROPYLENE STREAMS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none">Note: Concentration prep., vessel type, replication, test conditions.	<p>Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation.</p> <p>The Antoine Method is described in the <u>Handbook of Chemical Property Estimation</u>, Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.</p> <p>A modified Grain Method is described on page 31 of Neely and Blau's <u>Environmental Exposure from Chemicals</u>, Volume 1, CRC Press. 1985.</p>
Results: Units/Value: <ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	<p>Calculated and measured vapor pressure data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential vapor pressure range for substances represented by the two CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition.</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the vapor pressure range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p>

Vapor Pressure (Range)

CAS No.: 115-07-1; 68606-26-8
 Robust Summary No.: OP E462

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"> <thead> <tr> <th data-bbox="695 296 834 352">Substance Constituent</th> <th data-bbox="943 296 1110 352">Calculated VP (hPa @ 25°C)</th> <th data-bbox="1182 296 1349 352">Measured* VP (hPa @ 25°C)</th> </tr> </thead> <tbody> <tr> <td data-bbox="695 384 834 411">propadiene</td> <td data-bbox="987 384 1066 411">6.71 E³</td> <td data-bbox="1226 384 1305 411">7.24 E³</td> </tr> <tr> <td data-bbox="695 415 813 443">propylene</td> <td data-bbox="987 415 1066 443">9.31 E³</td> <td data-bbox="1226 415 1305 443">1.16 E⁴</td> </tr> <tr> <td data-bbox="695 447 792 474">propane</td> <td data-bbox="987 447 1066 474">8.19 E³</td> <td data-bbox="1226 447 1305 474">9.53 E³</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)	propadiene	6.71 E ³	7.24 E ³	propylene	9.31 E ³	1.16 E ⁴	propane	8.19 E ³	9.53 E ³
Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)											
propadiene	6.71 E ³	7.24 E ³											
propylene	9.31 E ³	1.16 E ⁴											
propane	8.19 E ³	9.53 E ³											
<p>Test Substance:</p>	<p>The Propylene Streams Category includes the following CAS numbers:</p> <p>115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p>Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p>More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>												
<p>Conclusion:</p>	<p>Based on calculated constituent data, substances in this category can have a vapor pressure range of 6.71 E³ to 9.31 E³ hPa @ 25°C. Based on measured constituent data, substances in this category can have a vapor pressure range of 7.24 E³ to 1.16 E⁴ hPa @ 25°C.</p>												

Vapor Pressure (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E462

Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the two CAS numbers listed under <u>Test Substance</u> . This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Water Solubility (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.:OP E464

PROPYLENE STREAMS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 115-07-1; 68606-26-8]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: <ul style="list-style-type: none">Note: Concentration prep., vessel type, replication, test conditions.	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". <i>Environ. Toxicol. Chem.</i> 15:100-106. 1995.
Results: Units/Value: <ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	<p>Calculated and measured water solubility data for representative constituents of the Propylene Streams Category are listed below. The data identify a potential water range for substances represented by the two CAS numbers under <u>Test Substance</u>. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water).</p> <p>Commercial substances in this category consist of both high purity hydrocarbons and isolated intermediates with a carbon number distribution that is predominantly C3. The three chemicals selected to represent the water solubility range of this category are C3 hydrocarbons that can be found in substances identified by the two CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.</p>

Water Solubility (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.: OP E464

<p>Results: (continued)</p> <p>Units/Value:</p> <p>Note: Deviations from protocol or guideline, analytical method.</p>	<table border="1"><thead><tr><th data-bbox="695 296 834 352">Substance Constituent</th><th data-bbox="915 296 1094 352">Calculated WS (mg/L @ 25°C)</th><th data-bbox="1154 296 1333 352">Measured WS* (mg/L @ 25°C)</th></tr></thead><tbody><tr><td data-bbox="695 386 834 413">propadiene</td><td data-bbox="972 386 1037 413">1449</td><td data-bbox="1182 386 1247 413">2147</td></tr><tr><td data-bbox="695 417 818 445">propylene</td><td data-bbox="972 417 1037 445">1162</td><td data-bbox="1198 417 1247 445">200</td></tr><tr><td data-bbox="695 449 797 476">propane</td><td data-bbox="972 449 1037 476">1088</td><td data-bbox="1198 449 1279 476">368.9</td></tr></tbody></table> <p data-bbox="695 506 1442 625">* Experimental values from EPIWIN database. The data represent a potential water solubility range for substances represented by the two CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)	propadiene	1449	2147	propylene	1162	200	propane	1088	368.9
Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)											
propadiene	1449	2147											
propylene	1162	200											
propane	1088	368.9											
<p>Test Substance:</p>	<p data-bbox="695 678 1414 735">The Propylene Streams Category includes the following CAS numbers:</p> <p data-bbox="695 785 1078 842">115-07-1 1-Propene 68606-26-8 Hydrocarbons, C3</p> <p data-bbox="695 877 1474 1056">Propylene Streams Category substances arise from production processes associated with ethylene manufacturing. The two CAS numbers are used to describe the four process streams that are commercial products or isolated intermediates. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3.</p> <p data-bbox="695 1092 1458 1178">More information on the Propylene Streams Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <p data-bbox="695 1245 1474 1392">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Propylene Streams Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>												
<p>Conclusion:</p>	<p data-bbox="695 1413 1474 1530">Based on calculated constituent data, substances in this category can have a water solubility range of 1088 to 1449 mg/L @ 25°C. Based on measured constituent data, substances in this category can have a water solubility range of 200 to 2147 mg/L @ 25°C.</p>												

Water Solubility (Range)

CAS No.: 115-07-1; 68606-26-8

Robust Summary No.:OP E464

Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the two CAS numbers listed under <u>Test Substance</u> . This robust summary has a reliability rating of 2 because the data are not for specific substances in the Propylene Streams Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Water Solubility. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.