

Boiling Point (Range)

201-15050B

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-
55-8; 78-79-5

Robust Summary No.: OP E360

C5 NON-CYCLICS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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 C5 Non-Cyclics Category are listed below. The data identify a potential boiling point range for substances represented by the 15 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the boiling point range of this category are C5 hydrocarbons that can be found in substances identified by the 15 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>

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<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="683 352 922 415">Substance Constituent</th> <th data-bbox="922 352 1161 415">Calculated BP (°C)</th> <th data-bbox="1161 352 1472 415">Measured* BP (°C)</th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>27.82</td> <td>0.8</td> </tr> <tr> <td>cis-pentene-2</td> <td>53.97</td> <td>36.3</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>28.20</td> <td>20.1</td> </tr> <tr> <td>1,4-pentadiene</td> <td>42.12</td> <td>26.0</td> </tr> <tr> <td>Isopentane</td> <td>30.18</td> <td>27.8</td> </tr> <tr> <td>Isoprene</td> <td>34.95</td> <td>34.0</td> </tr> <tr> <td>n-pentane</td> <td>46.01</td> <td>36.0</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>46.92</td> <td>38.5</td> </tr> <tr> <td>cyclopentene</td> <td>65.86</td> <td>44.2</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the 15 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated BP (°C)	Measured* BP (°C)	cis-butene-2	27.82	0.8	cis-pentene-2	53.97	36.3	3-methyl-1-butene	28.20	20.1	1,4-pentadiene	42.12	26.0	Isopentane	30.18	27.8	Isoprene	34.95	34.0	n-pentane	46.01	36.0	2-methyl-2-butene	46.92	38.5	cyclopentene	65.86	44.2
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<p>Test Substance:</p>	<p>The C5 Non-Cyclics Category includes the following CAS numbers:</p> <table border="1"> <tbody> <tr> <td>513-35-9</td> <td>2-Butene, 2-methyl-</td> </tr> <tr> <td>64742-83-2</td> <td>Naphtha, petroleum, light steam-cracked</td> </tr> <tr> <td>68410-97-9</td> <td>Distillates, petroleum, light distillate hydrotreating process, low-boiling</td> </tr> <tr> <td>68476-43-7</td> <td>Hydrocarbons, C4-6, C5-rich</td> </tr> <tr> <td>68476-55-1</td> <td>Hydrocarbons, C5-rich</td> </tr> <tr> <td>68477-35-0</td> <td>Distillates, petroleum, C3-6, piperylene-rich</td> </tr> <tr> <td>68514-39-6</td> <td>Naphtha, petroleum, light steam-cracked, isoprene-rich</td> </tr> <tr> <td>68527-11-7</td> <td>Alkenes, C5</td> </tr> <tr> <td>68527-19-5</td> <td>Hydrocarbons, C1-4, debutanizer fraction</td> </tr> <tr> <td>68603-00-9</td> <td>Distillates, petroleum, thermal cracked naphtha and gas oil</td> </tr> <tr> <td>68603-03-2</td> <td>Distillates, petroleum, thermal cracked naphtha and gas oil, extractive</td> </tr> <tr> <td>68606-29-1</td> <td>Hydrocarbons, C4 and C8, butene concentrator by-product</td> </tr> <tr> <td>68606-36-0</td> <td>Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product</td> </tr> <tr> <td>68956-55-8</td> <td>Hydrocarbons, C5-unsatd.</td> </tr> <tr> <td>78-79-5</td> <td>1,3-Butadiene, 2-methyl-</td> </tr> </tbody> </table> <p>C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes. The process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p>	513-35-9	2-Butene, 2-methyl-	64742-83-2	Naphtha, petroleum, light steam-cracked	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68476-43-7	Hydrocarbons, C4-6, C5-rich	68476-55-1	Hydrocarbons, C5-rich	68477-35-0	Distillates, petroleum, C3-6, piperylene-rich	68514-39-6	Naphtha, petroleum, light steam-cracked, isoprene-rich	68527-11-7	Alkenes, C5	68527-19-5	Hydrocarbons, C1-4, debutanizer fraction	68603-00-9	Distillates, petroleum, thermal cracked naphtha and gas oil	68603-03-2	Distillates, petroleum, thermal cracked naphtha and gas oil, extractive	68606-29-1	Hydrocarbons, C4 and C8, butene concentrator by-product	68606-36-0	Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product	68956-55-8	Hydrocarbons, C5-unsatd.	78-79-5	1,3-Butadiene, 2-methyl-
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	<p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>Based on calculated constituent data, substances in this category can have a boiling range of 27.82 to 65.86°C @ 760 mm Hg. Based on measured constituent data, substances in this category can have a boiling range of 0.8 to 44.2°C @ 760 mm Hg.</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 boiling point range for substances represented by the 15 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 C5 Non-Cyclics 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>
Reference:	<p>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.)</p>
Other (source):	<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 Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Photodegradation (Direct)

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C5 NON-CYCLICS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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 C5 Non-Cyclics Category (C5 refers to a chemical with 5 carbons). The C5 Non-Cyclics Category includes ten process streams:</p> <ul style="list-style-type: none">• Pyrolysis C5s• Hydrotreated C5s• Pentenes• Piperylene Concentrate• Isoprene Concentrate• Isoprene-Piperylene Concentrate

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	<ul style="list-style-type: none">• Isoprene, High Purity• 2-Methyl-2-Butene• Metathesis Byproduct <p>Fifteen 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 C5 Non-Cyclics 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 consist of both high purity hydrocarbons and complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes (with the exception of the Metathesis Byproduct stream which has 51% hexenes) and predominantly non-cyclic. All but two of these streams contain isoprene. The two streams without isoprene contain components such as 2-methyl-2-butene and pentenes, which are found in other streams in the category. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>C5 Non-Cyclics</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>C5 Non-Cyclics streams arise from production processes associated with ethylene manufacturing. More information on the C5 Non-Cyclics 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 ten process streams in this category are:</p> <ul style="list-style-type: none">• Pyrolysis C5s consist of a hydrocarbon distillate fraction separated from pyrolysis gasoline (the C5+ portion of the cracked gas in the ethylene process). The carbon number distribution of the product is predominantly C5, but the stream also typically contains relatively low levels of the higher boiling C4 substances (e.g. 1,2-butadiene) as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 0.25% and present in the distillate largely due to azeotropes of benzene with other hydrocarbon species in the complex mixture. The 1,3-butadiene content is typically 1%. The stream contains significant levels of olefins, diolefins and cyclics.
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	<ul style="list-style-type: none">• Hydrotreated C5s result from hydrogenation of Pyrolysis C5s over catalyst. Typically the stream that is charged to the hydrogenation reactor is a broader boiling range stream than the C5 fraction. For example, a full range pyrolysis gasoline may be hydrotreated and the resulting product then fractionated to produce the Hydrotreated C5s as a distillate fraction. The hydrogenation process may be either a one-stage or two-stage process. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to monoolefins. The two-stage process is typically a vapor-phase, more severe hydrogenation that converts monoolefins to paraffins. Typically, Hydrotreated C5s are subject only to one-stage hydrogenation because the product is intended for use in gasoline where the monoolefins are desired components. Similar to Pyrolysis C5s, Hydrotreated C5s have a carbon number distribution that is predominantly C5, and contain low levels of the higher boiling C4 substances as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 1%. Unlike pyrolysis C5s, the diolefin content in Hydrotreated C5s is very low.• Pentenenes is the distillate that is sometimes removed during the fractionation of Pyrolysis C5s into concentrates of the reactive diolefins: isoprene, piperylene (1,3-pentadiene) and cyclopentadiene (as dimer). The stream has a carbon number distribution that is predominantly C4-C5, consisting in part of isopentane and the more volatile pentenes such as 1-pentene, with about 1-3% isoprene. The stream typically contains the C4 compounds that were present in the Pyrolysis C5s, including 1,3-butadiene. Alternately, Pentenes can be removed later in the processing, for example by distillation of the Isoprene Concentrate.• Piperylene Concentrate is produced from Pyrolysis C5s by first "heat soaking" the stream in order to dimerize 1,3-cyclopentadiene (CPD). The heat soak produces a mixture of CPD dimer and codimers (DCPD Concentrate) that can be removed as a bottoms product from the balance of the Pyrolysis C5 stream. After removal of the DCPD Concentrate, what is left of the Pyrolysis C5s can be charged to a distillation column (the isoprene-piperylene splitter) to yield Piperylene Concentrate as a bottoms product. The carbon number distribution for Piperylene Concentrate is predominantly C5. A typical Piperylene Concentrate stream composition includes 60% piperylenes, 10% 2-methyl-2-butene, and about 0.2% benzene.• Isoprene Concentrate is also a distillate of the isoprene-piperylene splitter described above. The carbon number distribution is predominantly C5. A typical Isoprene Concentrate stream contains 40% isoprene with the balance largely iso- and n-pentane and C5 monoolefins. Pentenes, as described for the Pentenes stream, may or may not have been removed in the
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	<p>distillation sequence and this has the corresponding effect on the concentration of the lower pentene and pentane components in the Isoprene Concentrate.</p> <ul style="list-style-type: none">• Isoprene-Piperylene Concentrate refers to the intermediate process stream charged to the isoprene-piperylene splitter (as described above for piperylene concentrate) and is sometimes isolated as a product. This stream typically contains about 20% isoprene and 14% piperylenes.• Isoprene, High Purity (98+%) is produced by separation from isoprene concentrate. This is accomplished using an extractive distillation process.• Isoprene Purification Byproduct is a byproduct from the Isoprene purification process. The carbon number of the stream is predominantly C5 and the composition is largely iso- and n-pentane, plus lesser amounts of pentenes and about 5% isoprene. The byproduct may also contain 1,3-butadiene at about 0.5%.• 2-Methyl-2-Butene as a component is sometimes separated from a mixed C5 stream by first converting to an intermediate, then separating the intermediate from the mix by distillation, and then cracking the intermediate back to yield product 2-methyl-2-butene.• Metathesis Byproduct refers to the byproduct that results from the Metathesis process, sometimes included in an olefins plant, which converts ethylene and/or butenes into propylene. The stream is a gasoline stream consisting primarily of C5 and C6 olefins. <p><u>Photolysis of Hydrocarbons</u></p> <p>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.</p> <p>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.</p> <p>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</p>
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	<p>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.</p> <p>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):</p> <table border="1" data-bbox="610 716 1385 884"> <thead> <tr> <th rowspan="2"><u>Hydrocarbon</u></th> <th colspan="2"><u>l below 290 nm</u></th> <th colspan="2"><u>l above 290 nm</u></th> </tr> <tr> <th><u>λ_{max}</u></th> <th><u>ϵ</u></th> <th><u>λ_{max}</u></th> <th><u>ϵ</u></th> </tr> </thead> <tbody> <tr> <td>Ethylene</td> <td>193</td> <td>10,000</td> <td>-</td> <td>-</td> </tr> <tr> <td>1,3-Butadiene</td> <td>217</td> <td>2,090</td> <td>-</td> <td>-</td> </tr> <tr> <td>Benzene</td> <td>255</td> <td>215</td> <td>-</td> <td>-</td> </tr> </tbody> </table> <p>Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the C5 Non-Cyclics 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).</p> <p>Substances in the C5 Non-Cyclics 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.</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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, 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. 	<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	-	-
<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>																					
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1,3-Butadiene	217	2,090	-	-																					
Benzene	255	215	-	-																					
<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>																								

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Robust Summary No.: OP E368

Degradation Products**: • Note: Identification, concentration	Unknown
Test Substance:	The C5 Non-Cyclics Category includes the following CAS numbers: 513-35-9 2-Butene, 2-methyl- 64742-83-2 Naphtha, petroleum, light steam-cracked 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68476-43-7 Hydrocarbons, C4-6, C5-rich 68476-55-1 Hydrocarbons, C5-rich 68477-35-0 Distillates, petroleum, C3-6, piperylene-rich 68514-39-6 Naphtha, petroleum, light steam-cracked, isoprene-rich 68527-11-7 Alkenes, C5 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68603-00-9 Distillates, petroleum, thermal cracked naphtha and gas oil 68603-03-2 Distillates, petroleum, thermal cracked naphtha and gas oil, extractive 68606-29-1 Hydrocarbons, C4 and C8, butene concentrator by-product 68606-36-0 Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product 68956-55-8 Hydrocarbons, C5-unsatd. 78-79-5 1,3-Butadiene, 2-methyl-
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the C5 Non-Cyclics Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2002. Photodegradation (Direct): C5 Non-Cyclics 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 Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8;
78-79-5

Robust Summary No.: OP E367

C5 NON-CYCLICS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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:	The C5 Non-Cyclics Category includes the following CAS numbers: 513-35-9 2-Butene, 2-methyl- 64742-83-2 Naphtha, petroleum, light steam-cracked 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68476-43-7 Hydrocarbons, C4-6, C5-rich 68476-55-1 Hydrocarbons, C5-rich 68477-35-0 Distillates, petroleum, C3-6, piperylene-rich 68514-39-6 Naphtha, petroleum, light steam-cracked, isoprene-rich 68527-11-7 Alkenes, C5 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68603-00-9 Distillates, petroleum, thermal cracked naphtha and gas oil

Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E367

	<p>68603-03-2 Distillates, petroleum, thermal cracked naphtha and gas oil, extractive</p> <p>68606-29-1 Hydrocarbons, C4 and C8, butene concentrator by-product</p> <p>68606-36-0 Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product</p> <p>68956-55-8 Hydrocarbons, C5-unsatd.</p> <p>78-79-5 1,3-Butadiene, 2-methyl-</p> <p>C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes. The process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p> <p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics 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 chemicals in the C5 Non-Cyclics Category (C5 refers to a chemical with 5 carbons). The C5 Non-Cyclics Category includes ten process streams:</p> <ul style="list-style-type: none">• Pyrolysis C5s• Hydrotreated C5s• Pentenes• Piperylene Concentrate• Isoprene Concentrate• Isoprene-Piperylene Concentrate• Isoprene, High Purity• 2-Methyl-2-Butene• Metathesis Byproduct <p>Fifteen 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>

Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E367

	<p><u>The C5 Non-Cyclics 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 consist of both high purity hydrocarbons and complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes (with the exception of the Metathesis Byproduct stream which has 51% hexenes) and predominantly non-cyclic. All but two of these streams contain isoprene. The two streams without isoprene contain components such as 2-methyl-2-butene and pentenes, which are found in other streams in the category. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>C5 Non-Cyclics</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>C5 Non-Cyclics streams arise from production processes associated with ethylene manufacturing. More information on the C5 Non-Cyclics 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 ten process streams in this category are:</p> <ul style="list-style-type: none">• Pyrolysis C5s consist of a hydrocarbon distillate fraction separated from pyrolysis gasoline (the C5+ portion of the cracked gas in the ethylene process). The carbon number distribution of the product is predominantly C5, but the stream also typically contains relatively low levels of the higher boiling C4 substances (e.g. 1,2-butadiene) as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 0.25% and present in the distillate largely due to azeotropes of benzene with other hydrocarbon species in the complex mixture. The 1,3-butadiene content is typically 1%. The stream contains significant levels of olefins, diolefins and cyclics.• Hydrotreated C5s result from hydrogenation of Pyrolysis C5s over catalyst. Typically the stream that is charged to the hydrogenation reactor is a broader boiling range stream than the C5 fraction. For example, a full range pyrolysis gasoline may be hydrotreated and the resulting product then fractionated to produce the Hydrotreated C5s as a distillate fraction. The hydrogenation process may be either a one-stage or two-stage process. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to monoolefins. The two-stage process is typically a vapor-phase, more severe hydrogenation that converts
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Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E367

	<p>monoolefins to paraffins. Typically, Hydrotreated C5s are subject only to one-stage hydrogenation because the product is intended for use in gasoline where the monoolefins are desired components. Similar to Pyrolysis C5s, Hydrotreated C5s have a carbon number distribution that is predominantly C5, and contain low levels of the higher boiling C4 substances as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 1%. Unlike pyrolysis C5s, the diolefin content in Hydrotreated C5s is very low.</p> <ul style="list-style-type: none">• Pentenenes is the distillate that is sometimes removed during the fractionation of Pyrolysis C5s into concentrates of the reactive diolefins: isoprene, piperylene (1,3-pentadiene) and cyclopentadiene (as dimer). The stream has a carbon number distribution that is predominantly C4-C5, consisting in part of isopentane and the more volatile pentenes such as 1-pentene, with about 1-3% isoprene. The stream typically contains the C4 compounds that were present in the Pyrolysis C5s, including 1,3-butadiene. Alternately, Penetenenes can be removed later in the processing, for example by distillation of the Isoprene Concentrate.• Piperylene Concentrate is produced from Pyrolysis C5s by first "heat soaking" the stream in order to dimerize 1,3-cyclopentadiene (CPD). The heat soak produces a mixture of CPD dimer and codimers (DCPD Concentrate) that can be removed as a bottoms product from the balance of the Pyrolysis C5 stream. After removal of the DCPD Concentrate, what is left of the Pyrolysis C5s can be charged to a distillation column (the isoprene-piperylene splitter) to yield Piperylene Concentrate as a bottoms product. The carbon number distribution for Piperylene Concentrate is predominantly C5. A typical Piperylene Concentrate stream composition includes 60% piperylenes, 10% 2-methyl-2-butene, and about 0.2% benzene.• Isoprene Concentrate is also a distillate of the isoprene-piperylene splitter described above. The carbon number distribution is predominantly C5. A typical Isoprene Concentrate stream contains 40% isoprene with the balance largely iso- and n-pentane and C5 monoolefins. Pentenes, as described for the Pentenes stream, may or may not have been removed in the distillation sequence and this has the corresponding effect on the concentration of the lower pentene and pentane components in the Isoprene Concentrate.• Isoprene-Piperylene Concentrate refers to the intermediate process stream charged to the isoprene-piperylene splitter (as described above for piperylene concentrate) and is sometimes isolated as a product. This stream typically contains about 20% isoprene and 14% piperylenes.
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Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E367

	<ul style="list-style-type: none">• Isoprene, High Purity (98+%) is produced by separation from isoprene concentrate. This is accomplished using an extractive distillation process.• Isoprene Purification Byproduct is a byproduct from the Isoprene purification process. The carbon number of the stream is predominantly C5 and the composition is largely iso- and n-pentane, plus lesser amounts of pentenes and about 5% isoprene. The byproduct may also contain 1,3-butadiene at about 0.5%.• 2-Methyl-2-Butene as a component is sometimes separated from a mixed C5 stream by first converting to an intermediate, then separating the intermediate from the mix by distillation, and then cracking the intermediate back to yield product 2-methyl-2-butene.• Metathesis Byproduct refers to the byproduct that results from the Metathesis process, sometimes included in an olefins plant, which converts ethylene and/or butenes into propylene. The stream is a gasoline stream consisting primarily of C5 and C6 olefins. <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 C5 Non-Cyclics 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 C5 Non-Cyclics Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of</p>
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Hydrolysis (Stability in Water)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E367

	<p>chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the C5 Non-Cyclics Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.</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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.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 C5 Non-Cyclics Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: C5 Non-Cyclics 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.

Photodegradation (Indirect)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-
55-8; 78-79-5

Robust Summary No.: OP E370

C5 NON-CYCLICS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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: 1.5×10^6 OH radicals/cm ³
Direct Photolysis**: Results: half-life, % degradation, quantum yield	Not applicable

Photodegradation (Indirect)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E370

<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 C5 Non-Cyclics Category</u></p> <p>C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes.</p> <p>Commercial products in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>C5 Non-Cyclics</u>.</p> <p>The nine chemicals selected to represent the atmospheric oxidation potential of this category are C5 hydrocarbons that can be found in substances identified by the 15 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>
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Photodegradation (Indirect)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-
55-8; 78-79-5

Robust Summary No.: OP E370

<p>Indirect Photolysis**: (cont'd)</p> <p>Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</p>	<table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Calculated* half-life (hrs)</u></th> <th><u>OH- Rate Constant (cm³/molecule-sec)</u></th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>2.3</td> <td>56.7 E⁻¹²</td> </tr> <tr> <td>cis-pentene-2</td> <td>2.2</td> <td>57.6 E⁻¹²</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>4.5</td> <td>28.6 E⁻¹²</td> </tr> <tr> <td>1,4-pentadiene</td> <td>2.4</td> <td>53.5 E⁻¹²</td> </tr> <tr> <td>Isopentane</td> <td>31.8</td> <td>4.0 E⁻¹²</td> </tr> <tr> <td>Isoprene</td> <td>1.2</td> <td>105.1 E⁻¹²</td> </tr> <tr> <td>n-pentane</td> <td>31.7</td> <td>4.0 E⁻¹²</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>1.5</td> <td>87.3 E⁻¹²</td> </tr> <tr> <td>cyclopentene</td> <td>2.2</td> <td>58.8 E⁻¹²</td> </tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p> <p>More information on the C5 Non-Cyclics 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. <i>J. Phys. Chem. Ref. Data Monograph No. 1</i>, 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 	<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>	cis-butene-2	2.3	56.7 E ⁻¹²	cis-pentene-2	2.2	57.6 E ⁻¹²	3-methyl-1-butene	4.5	28.6 E ⁻¹²	1,4-pentadiene	2.4	53.5 E ⁻¹²	Isopentane	31.8	4.0 E ⁻¹²	Isoprene	1.2	105.1 E ⁻¹²	n-pentane	31.7	4.0 E ⁻¹²	2-methyl-2-butene	1.5	87.3 E ⁻¹²	cyclopentene	2.2	58.8 E ⁻¹²
<u>Chemical</u>	<u>Calculated* half-life (hrs)</u>	<u>OH- Rate Constant (cm³/molecule-sec)</u>																													
cis-butene-2	2.3	56.7 E ⁻¹²																													
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Isoprene	1.2	105.1 E ⁻¹²																													
n-pentane	31.7	4.0 E ⁻¹²																													
2-methyl-2-butene	1.5	87.3 E ⁻¹²																													
cyclopentene	2.2	58.8 E ⁻¹²																													
<p>Degradation Products**:</p> <ul style="list-style-type: none"> • Note: Identification, concentration 	<p>Unknown</p>																														

Photodegradation (Indirect)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E370

Test Substance:	The C5 Non-Cyclics Category includes the following CAS numbers: 513-35-9 2-Butene, 2-methyl- 64742-83-2 Naphtha, petroleum, light steam-cracked 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68476-43-7 Hydrocarbons, C4-6, C5-rich 68476-55-1 Hydrocarbons, C5-rich 68477-35-0 Distillates, petroleum, C3-6, piperylene-rich 68514-39-6 Naphtha, petroleum, light steam-cracked, isoprene-rich 68527-11-7 Alkenes, C5 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68603-00-9 Distillates, petroleum, thermal cracked naphtha and gas oil 68603-03-2 Distillates, petroleum, thermal cracked naphtha and gas oil, extractive 68606-29-1 Hydrocarbons, C4 and C8, butene concentrator by-product 68606-36-0 Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product 68956-55-8 Hydrocarbons, C5-unsatd. 78-79-5 1,3-Butadiene, 2-methyl-
Conclusion:	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 1.2 to 31.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions 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 15 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 C5 Non-Cyclics 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.

Photodegradation (Indirect)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-
55-8; 78-79-5

Robust Summary No.: OP E370

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

Partition Coefficient (Range)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E363

C5 NON-CYCLICS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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.	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.
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 C5 Non-Cyclics Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 15 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the log K_{ow} range of this category are C5 hydrocarbons can be found in substances identified by the 15 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.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E363

<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="683 352 829 415">Substance Constituent</th> <th data-bbox="829 352 1101 415">Calculated log K_{ow} @ 25°C</th> <th data-bbox="1101 352 1472 415">Measured* log K_{ow} @ 25°C</th> </tr> </thead> <tbody> <tr> <td data-bbox="683 443 829 470">cis-butene-2</td> <td data-bbox="829 443 1101 470">2.09</td> <td data-bbox="1101 443 1472 470">2.31</td> </tr> <tr> <td data-bbox="683 470 829 497">cis-pentene-2</td> <td data-bbox="829 470 1101 497">2.58</td> <td data-bbox="1101 470 1472 497">na</td> </tr> <tr> <td data-bbox="683 497 829 525">3-methyl-1-butene</td> <td data-bbox="829 497 1101 525">2.59</td> <td data-bbox="1101 497 1472 525">na</td> </tr> <tr> <td data-bbox="683 525 829 552">1,4-pentadiene</td> <td data-bbox="829 525 1101 552">2.52</td> <td data-bbox="1101 525 1472 552">2.48</td> </tr> <tr> <td data-bbox="683 552 829 579">Isopentane</td> <td data-bbox="829 552 1101 579">2.72</td> <td data-bbox="1101 552 1472 579">na</td> </tr> <tr> <td data-bbox="683 579 829 606">Isoprene</td> <td data-bbox="829 579 1101 606">2.58</td> <td data-bbox="1101 579 1472 606">2.42</td> </tr> <tr> <td data-bbox="683 606 829 634">n-pentane</td> <td data-bbox="829 606 1101 634">2.80</td> <td data-bbox="1101 606 1472 634">3.39</td> </tr> <tr> <td data-bbox="683 634 829 661">2-methyl-2-butene</td> <td data-bbox="829 634 1101 661">2.64</td> <td data-bbox="1101 634 1472 661">2.67</td> </tr> <tr> <td data-bbox="683 661 829 688">cyclopentene</td> <td data-bbox="829 661 1101 688">2.47</td> <td data-bbox="1101 661 1472 688">na</td> </tr> </tbody> </table> <p data-bbox="683 743 1472 863">* Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the 15 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C	cis-butene-2	2.09	2.31	cis-pentene-2	2.58	na	3-methyl-1-butene	2.59	na	1,4-pentadiene	2.52	2.48	Isopentane	2.72	na	Isoprene	2.58	2.42	n-pentane	2.80	3.39	2-methyl-2-butene	2.64	2.67	cyclopentene	2.47	na
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<p>Test Substance:</p>	<p>The C5 Non-Cyclics Category includes the following CAS numbers:</p> <table border="1"> <tbody> <tr> <td data-bbox="683 961 829 989">513-35-9</td> <td data-bbox="829 961 1472 989">2-Butene, 2-methyl-</td> </tr> <tr> <td data-bbox="683 989 829 1016">64742-83-2</td> <td data-bbox="829 989 1472 1016">Naphtha, petroleum, light steam-cracked</td> </tr> <tr> <td data-bbox="683 1016 829 1043">68410-97-9</td> <td data-bbox="829 1016 1472 1079">Distillates, petroleum, light distillate hydrotreating process, low-boiling</td> </tr> <tr> <td data-bbox="683 1079 829 1106">68476-43-7</td> <td data-bbox="829 1079 1472 1106">Hydrocarbons, C4-6, C5-rich</td> </tr> <tr> <td data-bbox="683 1106 829 1134">68476-55-1</td> <td data-bbox="829 1106 1472 1134">Hydrocarbons, C5-rich</td> </tr> <tr> <td data-bbox="683 1134 829 1161">68477-35-0</td> <td data-bbox="829 1134 1472 1161">Distillates, petroleum, C3-6, piperylene-rich</td> </tr> <tr> <td data-bbox="683 1161 829 1188">68514-39-6</td> <td data-bbox="829 1161 1472 1224">Naphtha, petroleum, light steam-cracked, isoprene-rich</td> </tr> <tr> <td data-bbox="683 1224 829 1251">68527-11-7</td> <td data-bbox="829 1224 1472 1251">Alkenes, C5</td> </tr> <tr> <td data-bbox="683 1251 829 1278">68527-19-5</td> <td data-bbox="829 1251 1472 1278">Hydrocarbons, C1-4, debutanizer fraction</td> </tr> <tr> <td data-bbox="683 1278 829 1306">68603-00-9</td> <td data-bbox="829 1278 1472 1341">Distillates, petroleum, thermal cracked naphtha and gas oil</td> </tr> <tr> <td data-bbox="683 1341 829 1369">68603-03-2</td> <td data-bbox="829 1341 1472 1404">Distillates, petroleum, thermal cracked naphtha and gas oil, extractive</td> </tr> <tr> <td data-bbox="683 1404 829 1432">68606-29-1</td> <td data-bbox="829 1404 1472 1467">Hydrocarbons, C4 and C8, butene concentrator by-product</td> </tr> <tr> <td data-bbox="683 1467 829 1495">68606-36-0</td> <td data-bbox="829 1467 1472 1530">Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product</td> </tr> <tr> <td data-bbox="683 1530 829 1558">68956-55-8</td> <td data-bbox="829 1530 1472 1558">Hydrocarbons, C5-unsatd.</td> </tr> <tr> <td data-bbox="683 1558 829 1585">78-79-5</td> <td data-bbox="829 1558 1472 1585">1,3-Butadiene, 2-methyl-</td> </tr> </tbody> </table> <p data-bbox="683 1629 1472 1869">C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes. The process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p>	513-35-9	2-Butene, 2-methyl-	64742-83-2	Naphtha, petroleum, light steam-cracked	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68476-43-7	Hydrocarbons, C4-6, C5-rich	68476-55-1	Hydrocarbons, C5-rich	68477-35-0	Distillates, petroleum, C3-6, piperylene-rich	68514-39-6	Naphtha, petroleum, light steam-cracked, isoprene-rich	68527-11-7	Alkenes, C5	68527-19-5	Hydrocarbons, C1-4, debutanizer fraction	68603-00-9	Distillates, petroleum, thermal cracked naphtha and gas oil	68603-03-2	Distillates, petroleum, thermal cracked naphtha and gas oil, extractive	68606-29-1	Hydrocarbons, C4 and C8, butene concentrator by-product	68606-36-0	Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product	68956-55-8	Hydrocarbons, C5-unsatd.	78-79-5	1,3-Butadiene, 2-methyl-
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Partition Coefficient (Range)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
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55-8; 78-79-5

Robust Summary No.: OP E363

	<p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>Based on calculated constituent data, substances in this category can have a log K_{ow} range of 2.09 to 2.80 @ 25°C. Based on measured constituent data, substances in this category can have a log K_{ow} range of 2.31 to 3.39 @ 25°C.</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 log K_{ow} range for substances represented by the 15 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 C5 Non-Cyclics 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>
Reference:	<p>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.)</p>
Other (source):	<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 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.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E361

C5 NON-CYCLICS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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 C5 Non-Cyclics Category are listed below. The data identify a potential melting point range for substances represented by the 15 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the melting point range of this category are C5 hydrocarbons that can be found in substances identified by the 15 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)

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Robust Summary No.: OP E361

<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 <u>Constituent</u></th> <th>Calculated <u>MP (°C)</u></th> <th>Measured* <u>MP (°C)</u></th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>-120.4</td> <td>-105.5</td> </tr> <tr> <td>cis-pentene-2</td> <td>-107.1</td> <td>-140.2</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>-120.5</td> <td>-168.5</td> </tr> <tr> <td>1,4-pentadiene</td> <td>-109.8</td> <td>-148.8</td> </tr> <tr> <td>Isopentane</td> <td>-119.0</td> <td>-159.9</td> </tr> <tr> <td>Isoprene</td> <td>-118.9</td> <td>-145.9</td> </tr> <tr> <td>n-pentane</td> <td>-106.9</td> <td>-129.7</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>-116.2</td> <td>-133.7</td> </tr> <tr> <td>cyclopentene</td> <td>-93.2</td> <td>-135.1</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the 15 CAS numbers under <u>Test Substance</u>.</p>	Substance <u>Constituent</u>	Calculated <u>MP (°C)</u>	Measured* <u>MP (°C)</u>	cis-butene-2	-120.4	-105.5	cis-pentene-2	-107.1	-140.2	3-methyl-1-butene	-120.5	-168.5	1,4-pentadiene	-109.8	-148.8	Isopentane	-119.0	-159.9	Isoprene	-118.9	-145.9	n-pentane	-106.9	-129.7	2-methyl-2-butene	-116.2	-133.7	cyclopentene	-93.2	-135.1
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Melting Point (Range)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E361

	<p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a melting range of -93.2 to -120.5 °C. Based on measured constituent data, substances in this category can have a melting range of -105.5 to -168.5°C.
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 melting point range for substances represented by the 15 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 C5 Non-Cyclics 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>
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.

Transport / Distribution (Fugacity)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E369

C5 NON-CYCLICS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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>

Transport / Distribution (Fugacity)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E369

<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 C5 Non-Cyclics Category are listed below. The data identify a potential distribution for substances represented by the 15 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the environmental distribution range of this category are C5 hydrocarbons that are common across the 15 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, and olefinic process (distillation) knowledge.</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"> <thead> <tr> <th rowspan="3"><u>Chemical</u></th> <th colspan="2"><u>Calculated*</u></th> <th colspan="2"><u>Measured**</u></th> </tr> <tr> <th colspan="2"><u>Percent Distribution</u></th> <th colspan="2"><u>Percent Distribution</u></th> </tr> <tr> <th><u>Air</u></th> <th><u>Water</u></th> <th><u>Air</u></th> <th><u>Water</u></th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>99.97</td> <td>0.03</td> <td>99.98</td> <td>0.02</td> </tr> <tr> <td>cis-pentene-2</td> <td>99.97</td> <td>0.03</td> <td>99.97</td> <td>0.03</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>99.98</td> <td>0.02</td> <td>99.98</td> <td>0.02</td> </tr> <tr> <td>1,4-pentadiene</td> <td>99.97</td> <td>0.02</td> <td>99.97</td> <td>0.02</td> </tr> <tr> <td>Isopentane</td> <td>99.98</td> <td>0.01</td> <td>99.98</td> <td>0.01</td> </tr> <tr> <td>Isoprene</td> <td>99.97</td> <td>0.02</td> <td>99.96</td> <td>0.03</td> </tr> <tr> <td>n-pentane</td> <td>99.97</td> <td>0.02</td> <td>99.99</td> <td>0.01</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>99.97</td> <td>0.03</td> <td>99.97</td> <td>0.02</td> </tr> <tr> <td>cyclopentene</td> <td>99.94</td> <td>0.04</td> <td>99.94</td> <td>0.04</td> </tr> </tbody> </table> <p>* Distribution values determined using calculated input data from EPIWIN program</p> <p>** Distribution values determined using input data from the EPIWIN program experimental database</p> <p>Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as 0.01% or less. 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>Chemical</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>	cis-butene-2	99.97	0.03	99.98	0.02	cis-pentene-2	99.97	0.03	99.97	0.03	3-methyl-1-butene	99.98	0.02	99.98	0.02	1,4-pentadiene	99.97	0.02	99.97	0.02	Isopentane	99.98	0.01	99.98	0.01	Isoprene	99.97	0.02	99.96	0.03	n-pentane	99.97	0.02	99.99	0.01	2-methyl-2-butene	99.97	0.03	99.97	0.02	cyclopentene	99.94	0.04	99.94	0.04
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Transport / Distribution (Fugacity)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E369

Test Substance:	<p>The C5 Non-Cyclics Category includes the following CAS numbers:</p> <table><tr><td>513-35-9</td><td>2-Butene, 2-methyl-</td></tr><tr><td>64742-83-2</td><td>Naphtha, petroleum, light steam-cracked</td></tr><tr><td>68410-97-9</td><td>Distillates, petroleum, light distillate hydrotreating process, low-boiling</td></tr><tr><td>68476-43-7</td><td>Hydrocarbons, C4-6, C5-rich</td></tr><tr><td>68476-55-1</td><td>Hydrocarbons, C5-rich</td></tr><tr><td>68477-35-0</td><td>Distillates, petroleum, C3-6, piperylene-rich</td></tr><tr><td>68514-39-6</td><td>Naphtha, petroleum, light steam-cracked, isoprene-rich</td></tr><tr><td>68527-11-7</td><td>Alkenes, C5</td></tr><tr><td>68527-19-5</td><td>Hydrocarbons, C1-4, debutanizer fraction</td></tr><tr><td>68603-00-9</td><td>Distillates, petroleum, thermal cracked naphtha and gas oil</td></tr><tr><td>68603-03-2</td><td>Distillates, petroleum, thermal cracked naphtha and gas oil, extractive</td></tr><tr><td>68606-29-1</td><td>Hydrocarbons, C4 and C8, butene concentrator by-product</td></tr><tr><td>68606-36-0</td><td>Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product</td></tr><tr><td>68956-55-8</td><td>Hydrocarbons, C5-unsatd.</td></tr><tr><td>78-79-5</td><td>1,3-Butadiene, 2-methyl-</td></tr></table> <p>C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes. The process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p> <p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.	513-35-9	2-Butene, 2-methyl-	64742-83-2	Naphtha, petroleum, light steam-cracked	68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling	68476-43-7	Hydrocarbons, C4-6, C5-rich	68476-55-1	Hydrocarbons, C5-rich	68477-35-0	Distillates, petroleum, C3-6, piperylene-rich	68514-39-6	Naphtha, petroleum, light steam-cracked, isoprene-rich	68527-11-7	Alkenes, C5	68527-19-5	Hydrocarbons, C1-4, debutanizer fraction	68603-00-9	Distillates, petroleum, thermal cracked naphtha and gas oil	68603-03-2	Distillates, petroleum, thermal cracked naphtha and gas oil, extractive	68606-29-1	Hydrocarbons, C4 and C8, butene concentrator by-product	68606-36-0	Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product	68956-55-8	Hydrocarbons, C5-unsatd.	78-79-5	1,3-Butadiene, 2-methyl-
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Transport / Distribution (Fugacity)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6;
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55-8; 78-79-5

Robust Summary No.: OP E369

Conclusion:	<p>The partitioning data represent a potential distribution range for substances in the 15 CAS numbers listed under <u>Test Substance</u>. Substances in the C5 Non-Cyclics 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>
Reliability:	<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 15 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 C5 Non-Cyclics 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>
Reference:	<p>Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.</p>
Other (source):	<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 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.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E362

C5 NON-CYCLICS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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 C5 Non-Cyclics Category are listed below. The data identify a potential vapor pressure range for substances represented by the 15 CAS numbers under Test Substance. 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the vapor pressure range of this category are C5 hydrocarbons that can be found in substances identified by the 15 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured</p>

Vapor Pressure (Range)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E362

	boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.																														
<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 VP (hPa @ 25°C)</th> <th>Measured* VP (hPa @ 25°C)</th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>2.31 E³</td> <td>2.33 E³</td> </tr> <tr> <td>cis-pentene-2</td> <td>6.76 E²</td> <td>6.75 E²</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>1.20 E³</td> <td>1.20 E³</td> </tr> <tr> <td>1,4-pentadiene</td> <td>9.79 E²</td> <td>9.97 E²</td> </tr> <tr> <td>Isopentane</td> <td>9.17 E²</td> <td>9.19 E²</td> </tr> <tr> <td>Isoprene</td> <td>7.35 E²</td> <td>7.33 E²</td> </tr> <tr> <td>n-pentane</td> <td>6.84 E²</td> <td>6.85 E²</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>6.24 E²</td> <td>6.24 E²</td> </tr> <tr> <td>cyclopentene</td> <td>5.06 E²</td> <td>5.06 E²</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 15 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)	cis-butene-2	2.31 E ³	2.33 E ³	cis-pentene-2	6.76 E ²	6.75 E ²	3-methyl-1-butene	1.20 E ³	1.20 E ³	1,4-pentadiene	9.79 E ²	9.97 E ²	Isopentane	9.17 E ²	9.19 E ²	Isoprene	7.35 E ²	7.33 E ²	n-pentane	6.84 E ²	6.85 E ²	2-methyl-2-butene	6.24 E ²	6.24 E ²	cyclopentene	5.06 E ²	5.06 E ²
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Vapor Pressure (Range)

CAS No.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E362

	<p>process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p> <p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>Based on calculated constituent data, substances in this category can have a vapor pressure range of 1.65 E^3 to 3.45 E^3 hPa @ 25°C. Based on measured constituent data, substances in this category can have a vapor pressure range of 1.68 E^3 to 3.08 E^3 hPa @ 25°C.</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 vapor pressure range for substances represented by the 15 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 C5 Non-Cyclics 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.</p>
Reference:	<p>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.)</p>
Other (source):	<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 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.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E364

C5 NON-CYCLICS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5]
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 C5 Non-Cyclics Category are listed below. The data identify a potential water solubility range for substances represented by the 15 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5. The nine chemicals selected to represent the water solubility range of this category are C5 hydrocarbons that can be found in substances identified by the 15 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.: 513-35-9; 64742-83-2; 68410-97-9; 68476-43-7; 68476-55-1; 68477-35-0; 68514-39-6; 68527-11-7; 68527-19-5; 68603-00-9; 68603-03-2; 68606-29-1; 68606-36-0; 68956-55-8; 78-79-5

Robust Summary No.: OP E364

<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 WS (mg/L @ 25°C)</th> <th>Measured WS* (mg/L @ 25°C)</th> </tr> </thead> <tbody> <tr> <td>cis-butene-2</td> <td>652.7</td> <td>423.5</td> </tr> <tr> <td>cis-pentene-2</td> <td>245.1</td> <td>na</td> </tr> <tr> <td>3-methyl-1-butene</td> <td>242.7</td> <td>na</td> </tr> <tr> <td>1,4-pentadiene</td> <td>278.2</td> <td>300.9</td> </tr> <tr> <td>Isopentane</td> <td>184.6</td> <td>na</td> </tr> <tr> <td>Isoprene</td> <td>247.2</td> <td>338.6</td> </tr> <tr> <td>n-pentane</td> <td>159.7</td> <td>49.8</td> </tr> <tr> <td>2-methyl-2-butene</td> <td>218.7</td> <td>206.1</td> </tr> <tr> <td>cyclopentene</td> <td>307.2</td> <td>na</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 15 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated WS (mg/L @ 25°C)	Measured WS* (mg/L @ 25°C)	cis-butene-2	652.7	423.5	cis-pentene-2	245.1	na	3-methyl-1-butene	242.7	na	1,4-pentadiene	278.2	300.9	Isopentane	184.6	na	Isoprene	247.2	338.6	n-pentane	159.7	49.8	2-methyl-2-butene	218.7	206.1	cyclopentene	307.2	na
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Robust Summary No.: OP E364

Test Substance: (cont'd)	<p>C5 Non-Cyclics Category substances arise from production processes associated with ethylene manufacturing. The 15 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated C5 processes. The process streams in this category consist of high purity hydrocarbons or complex hydrocarbon reaction products that are predominantly C5 alkanes or alkenes and predominantly non-cyclic.</p> <p>More information on the C5 Non-Cyclics 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 C5 Non-Cyclics Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	<p>Based on calculated constituent data, substances in this category can have a water solubility range of 159.7 to 652.7 mg/L @ 25°C. Based on measured constituent data, substances in this category can have a water solubility range of 49.8 to 423.5 mg/L @ 25°C.</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 water solubility range for substances represented by the 15 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 C5 Non-Cyclics 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.</p>
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