

Boiling Point (Range)

201-15104B

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E060

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FUEL OILS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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 Fuel Oils Category are listed below. The data identify a potential boiling point range for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the boiling point range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</p>

Boiling Point (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E060

<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 BP (°C)</th> <th>Measured* BP (°C)</th> </tr> </thead> <tbody> <tr> <td>indene</td> <td>212.89</td> <td>na</td> </tr> <tr> <td>dicyclopentadiene</td> <td>176.78</td> <td>170.0</td> </tr> <tr> <td>naphthalene</td> <td>231.64</td> <td>217.9</td> </tr> <tr> <td>methylnaphthalene</td> <td>249.60</td> <td>241.1</td> </tr> <tr> <td>1,1'-biphenyl</td> <td>272.53</td> <td>256.1</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential boiling point range for substances represented by the 12 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated BP (°C)	Measured* BP (°C)	indene	212.89	na	dicyclopentadiene	176.78	170.0	naphthalene	231.64	217.9	methylnaphthalene	249.60	241.1	1,1'-biphenyl	272.53	256.1						
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indene	212.89	na																							
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<p>Test Substance:</p>	<p>The Fuel Oils Category includes the following CAS numbers:</p> <table border="1"> <tbody> <tr> <td>64741-62-4</td> <td>Clarified oils, petroleum, catalytic cracked</td> </tr> <tr> <td>64742-90-1</td> <td>Residues, petroleum, steam cracked</td> </tr> <tr> <td>68131-05-5</td> <td>Hydrocarbon oils, process blends</td> </tr> <tr> <td>68409-73-4</td> <td>Aromatic hydrocarbons, biphenyl-rich</td> </tr> <tr> <td>68475-80-9</td> <td>Distillates, petroleum, light steam-cracked naphtha</td> </tr> <tr> <td>68513-69-9</td> <td>Residues, petroleum, steam cracked light</td> </tr> <tr> <td>68514-34-1</td> <td>Hydrocarbons, C9-14, ethylene-manufacture-by-product</td> </tr> <tr> <td>68527-18-4</td> <td>Gas oils, petroleum, steam-cracked</td> </tr> <tr> <td>68921-67-5</td> <td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td> </tr> <tr> <td>69013-21-4</td> <td>Fuel oil, pyrolysis</td> </tr> <tr> <td>69430-33-7</td> <td>Hydrocarbons, C6-30</td> </tr> <tr> <td>8002-05-9</td> <td>Petroleum</td> </tr> </tbody> </table> <p>The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of lower boiling materials. The 12 CAS numbers are used to describe the eight process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible.</p> <p>More information on the Fuel Oils 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 Fuel Oils Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 	64741-62-4	Clarified oils, petroleum, catalytic cracked	64742-90-1	Residues, petroleum, steam cracked	68131-05-5	Hydrocarbon oils, process blends	68409-73-4	Aromatic hydrocarbons, biphenyl-rich	68475-80-9	Distillates, petroleum, light steam-cracked naphtha	68513-69-9	Residues, petroleum, steam cracked light	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacture-by-product	68527-18-4	Gas oils, petroleum, steam-cracked	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	69013-21-4	Fuel oil, pyrolysis	69430-33-7	Hydrocarbons, C6-30	8002-05-9	Petroleum
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Robust Summary No.: OP E060

Conclusion:	The calculated boiling points for selected representative constituents that are present in category streams range from 176.78 to 272.53°C @ 760 mm Hg. The measured boiling points of these same constituents range from 170.0 to 256.1°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.
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 boiling point range for substances represented by the 12 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 Fuel Oils 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.
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 10/03)

* 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.

Photodegradation (Direct)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E068

FUEL OILS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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:	Not applicable
<ul style="list-style-type: none"> Wave length value (upper/lower) 	
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions:	Not applicable
<ul style="list-style-type: none"> Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol 	
Direct Photolysis**:	<p><u>Summary</u></p> <p>In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Fuel Oils Category. The Fuel Oils Category includes eight process streams:</p> <ul style="list-style-type: none"> Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit Light Pyrolysis Fuel Oil from the Ethylene Process Unit Quench Oil from the Ethylene Process Unit Water Quench System Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Gasoline Units

Photodegradation (Direct)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E068

	<ul style="list-style-type: none">• Hydrotreated Flux Oil• Biphenyl Concentrate <p>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 Fuel Oils Category</u></p> <p>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible. Twelve CAS numbers (see <u>Test Substance</u>) identify products derived from these process streams. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C8-C14. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Fuel Oils</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>More information on the Fuel Oils 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 eight process streams in this category are:</p> <ul style="list-style-type: none">• Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit: In ethylene plants cracking liquid feedstocks, the cracking furnace effluent (after heat recovery) is further quenched by injection of recycled quench oil. This step results in the condensation of higher boiling hydrocarbon compounds that are typically separated from the rest of the furnace effluent as the bottoms of the primary fractionation tower or oil quench tower. Lights are stripped from the excess oils generated from this quench system, resulting in the stream identified here as heavy pyrolysis fuel oil consisting of C10+ and considerable PAHs.• Light Pyrolysis Fuel Oil from the Ethylene Process Unit: In some cases, a light pyrolysis fuel oil is produced from the oil quench system in an ethylene plant that cracks liquid feedstocks. This stream may be produced as a side draw from the primary fractionation tower. The stream typically has a carbon number
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	<p>distribution of C9 to C14 and the major components are naphthalene (30 to 60%), methyl naphthalenes and other substituted one and two ring aromatics.</p> <ul style="list-style-type: none">• Quench Oil from the Ethylene Process Unit Water Quench System: In ethylene plants cracking only gases, the cracking furnace effluent (after heat recovery) may be further quenched with water. This step results in the condensation of a relatively small amount of higher boiling hydrocarbon components that, after stripping to remove lights, may be isolated as the Quench Oils from the Ethylene Process Unit Water Quench System. This stream is predominantly C7 through components boiling at 650°F or higher. The reported composition indicates 0.1% benzene, 5% toluene, 12% C8 aromatics, 5% naphthalene, 10% anthracene and 65% C7-C18 cyclic olefins.• Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation: This stream is separated by distillation from pyrolysis gasoline, as a bottoms product. The reported composition indicates a carbon number distribution of from C9 to hydrocarbons boiling at 650°F or higher. The reported typical composition includes 20% dicyclopentadiene, 30% codimers of C5 and C6 monomers, 20% naphthalene and substituted naphthalenes.• Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units: A single combined fuel oil stream for the ethylene process unit and the pyrolysis gasoline unit is not an uncommon situation for the industry. The carbon number distribution for this stream is generally C10 to compounds with a boiling point of 650°F or higher. At least in some cases, lower carbon number components are reported for the stream, e.g. C5s at approximately 2% and benzene at up to 4%. The major components reported in the stream are typically 25% C9 compounds, 10-47% naphthalene and 4-30% methylnaphthalenes.• Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Gasoline Units: Ethylene process operations that include both a pyrolysis gasoline distillation unit and a benzene hydrodealkylation unit may combine the fuel oil streams from these two units resulting in a single isolated product. Fuel oil is produced in the benzene HDA process by the HDA reactors and separated as a distillation bottoms product. The carbon number distribution for this combined fuel stream is C9 through hydrocarbons with a boiling point of 650°F or higher, although relatively low levels of lower carbon number hydrocarbons may be present, e.g. 0.2% benzene. The major components reported in the stream include 11% C9 aromatics to naphthalene, 7.5-12% DCPD, 7-13% naphthalene, 22% methylnaphthalenes, and 25-35% biphenyl.• Hydrotreated Flux Oil: is a hydrotreated fuel oil stream with a carbon number distribution predominantly C10 to hydrocarbons
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Photodegradation (Direct)

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Robust Summary No.: OP E068

with a boiling point of 650°F or higher. The stream may be produced as distillation bottoms from a pyrolysis gasoline hydrotreater unit. The components in the stream are predominantly aromatics, paraffins and cyclic compounds. This stream differs from the other fuel oils described above in that its diolefin and vinyl aromatic content is very low.

- **Biphenyl Concentrate:** is a co-product of the benzene hydrodealkylation unit that is isolated by distillation from the HDA reactor effluent. The carbon number distribution for the stream is C7 to C18, with the major component reported to be 65 to 95% biphenyl.

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):

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	λ below 290 nm		λ above 290 nm	
	<u>λ_{max}</u>	<u>ε</u>	<u>λ_{max}</u>	<u>ε</u>
<u>Hydrocarbon</u>				
Ethylene	193	10,000	-	-
Benzene	255	215	-	-
Biphenyl	246	20,000	-	-
Naphthalene	221	100,000	311	250
	270	5,000		
<p>Olefins with one double bond, or two conjugated double bonds, which constitute a significant proportion of the chemicals in the Fuel Oils Category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerization about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).</p> <p>Products in the Fuel Oils 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 Fuel Oils 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 	Not applicable			
<p>Degradation Products**:</p> <ul style="list-style-type: none"> • Note: Identification, concentration 	Unknown			

Photodegradation (Direct)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1;
68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E068

Test Substance:	The Fuel Oils Category includes the following CAS numbers: 64741-62-4 Clarified oils, petroleum, catalytic cracked 64742-90-1 Residues, petroleum, steam cracked 68131-05-5 Hydrocarbon oils, process blends 68409-73-4 Aromatic hydrocarbons, biphenyl-rich 68475-80-9 Distillates, petroleum, light steam-cracked naphtha 68513-69-9 Residues, petroleum, steam cracked light 68514-34-1 Hydrocarbons, C9-14, ethylene-manufacture-by-product 68527-18-4 Gas oils, petroleum, steam-cracked 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 69013-21-4 Fuel oil, pyrolysis 69430-33-7 Hydrocarbons, C6-30 8002-05-9 Petroleum
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the Fuel Oils Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): Fuel Oils Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 8/03)

* 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.

Transport / Distribution (Fugacity)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E069

FUEL OILS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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>

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Robust Summary No.: OP E069

<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 Fuel Oils Category are listed below. The data identify a potential distribution for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the environmental distribution range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure 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" data-bbox="690 1102 1388 1375"><thead><tr><th rowspan="2"><u>Chemical</u></th><th colspan="4"><u>Calculated*</u> <u>Percent Distribution</u></th></tr><tr><th><u>Air</u></th><th><u>Water</u></th><th><u>Soil</u></th><th><u>Sediment</u></th></tr></thead><tbody><tr><td>indene</td><td>47.61</td><td>31.05</td><td>20.86</td><td>0.46</td></tr><tr><td>dicyclopentadiene</td><td>98.00</td><td>0.87</td><td>1.11</td><td>0.02</td></tr><tr><td>naphthalene</td><td>24.47</td><td>32.28</td><td>42.28</td><td>0.94</td></tr><tr><td>methylnaphthalene</td><td>97.68</td><td>0.40</td><td>1.88</td><td>0.04</td></tr><tr><td>1,1'-biphenyl</td><td>10.06</td><td>14.48</td><td>73.77</td><td>1.64</td></tr></tbody></table> <p>* Distribution values determined using calculated input data from EPIWIN program</p>	<u>Chemical</u>	<u>Calculated*</u> <u>Percent Distribution</u>				<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	indene	47.61	31.05	20.86	0.46	dicyclopentadiene	98.00	0.87	1.11	0.02	naphthalene	24.47	32.28	42.28	0.94	methylnaphthalene	97.68	0.40	1.88	0.04	1,1'-biphenyl	10.06	14.48	73.77	1.64
<u>Chemical</u>	<u>Calculated*</u> <u>Percent Distribution</u>																																		
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1,1'-biphenyl	10.06	14.48	73.77	1.64																															

Transport / Distribution (Fugacity)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E069

<p>Results: (cont'd)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<p style="text-align: center;">Measured** <u>Percent Distribution</u></p> <table border="1"> <thead> <tr> <th><u>Chemical</u></th> <th><u>Air</u></th> <th><u>Water</u></th> <th><u>Soil</u></th> <th><u>Sediment</u></th> </tr> </thead> <tbody> <tr> <td>indene</td> <td>na</td> <td>na</td> <td>na</td> <td>na</td> </tr> <tr> <td>dicyclopentadiene</td> <td>98.55</td> <td>0.63</td> <td>0.80</td> <td>0.02</td> </tr> <tr> <td>naphthalene</td> <td>42.27</td> <td>20.56</td> <td>36.33</td> <td>0.81</td> </tr> <tr> <td>methylnaphthalene</td> <td>98.53</td> <td>0.19</td> <td>1.25</td> <td>0.03</td> </tr> <tr> <td>1,1'-biphenyl</td> <td>11.68</td> <td>9.15</td> <td>77.40</td> <td>1.72</td> </tr> </tbody> </table> <p>** Distribution values determined using input data from the EPIWIN program experimental database. na = not available</p>	<u>Chemical</u>	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>	indene	na	na	na	na	dicyclopentadiene	98.55	0.63	0.80	0.02	naphthalene	42.27	20.56	36.33	0.81	methylnaphthalene	98.53	0.19	1.25	0.03	1,1'-biphenyl	11.68	9.15	77.40	1.72
<u>Chemical</u>	<u>Air</u>	<u>Water</u>	<u>Soil</u>	<u>Sediment</u>																											
indene	na	na	na	na																											
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<p>Test Substance:</p>	<p>The Fuel Oils Category includes the following CAS numbers:</p> <table border="0"> <tr> <td>64741-62-4</td> <td>Clarified oils, petroleum, catalytic cracked</td> </tr> <tr> <td>64742-90-1</td> <td>Residues, petroleum, steam cracked</td> </tr> <tr> <td>68131-05-5</td> <td>Hydrocarbon oils, process blends</td> </tr> <tr> <td>68409-73-4</td> <td>Aromatic hydrocarbons, biphenyl-rich</td> </tr> <tr> <td>68475-80-9</td> <td>Distillates, petroleum, light steam-cracked naphtha</td> </tr> <tr> <td>68513-69-9</td> <td>Residues, petroleum, steam cracked light</td> </tr> <tr> <td>68514-34-1</td> <td>Hydrocarbons, C9-14, ethylene-manufacture-by-product</td> </tr> <tr> <td>68527-18-4</td> <td>Gas oils, petroleum, steam-cracked</td> </tr> <tr> <td>68921-67-5</td> <td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td> </tr> <tr> <td>69013-21-4</td> <td>Fuel oil, pyrolysis</td> </tr> <tr> <td>69430-33-7</td> <td>Hydrocarbons, C6-30</td> </tr> <tr> <td>8002-05-9</td> <td>Petroleum</td> </tr> </table> <p>The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of lower boiling materials. The 12 CAS numbers are used to describe the eight process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible.</p> <p>More information on the Fuel Oils 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 Fuel Oils Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 	64741-62-4	Clarified oils, petroleum, catalytic cracked	64742-90-1	Residues, petroleum, steam cracked	68131-05-5	Hydrocarbon oils, process blends	68409-73-4	Aromatic hydrocarbons, biphenyl-rich	68475-80-9	Distillates, petroleum, light steam-cracked naphtha	68513-69-9	Residues, petroleum, steam cracked light	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacture-by-product	68527-18-4	Gas oils, petroleum, steam-cracked	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	69013-21-4	Fuel oil, pyrolysis	69430-33-7	Hydrocarbons, C6-30	8002-05-9	Petroleum						
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Transport / Distribution (Fugacity)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E069

Conclusion:	<p>The partitioning data represent a potential distribution range for substances in the 12 CAS numbers listed under <u>Test Substance</u>. Substances in the Fuel Oils Category are complex hydrocarbon reaction products, and as a result, the potential environmental distribution of these substances is also expected to be complex. Constituent chemicals are calculated to partition either primarily to air or to air, water, and soil with a small percentage to sediment.</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 12 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 Fuel Oils 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 10/03)</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.

Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

FUEL OILS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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 Fuel Oils Category includes the following CAS numbers: 64741-62-4 Clarified oils, petroleum, catalytic cracked 64742-90-1 Residues, petroleum, steam cracked 68131-05-5 Hydrocarbon oils, process blends 68409-73-4 Aromatic hydrocarbons, biphenyl-rich 68475-80-9 Distillates, petroleum, light steam-cracked naphtha 68513-69-9 Residues, petroleum, steam cracked light 68514-34-1 Hydrocarbons, C9-14, ethylene-manufacture-by-product 68527-18-4 Gas oils, petroleum, steam-cracked 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 69013-21-4 Fuel oil, pyrolysis 69430-33-7 Hydrocarbons, C6-30 8002-05-9 Petroleum

Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

	<p>The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of some lower boiling materials. The 12 CAS numbers are used to describe the eight process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the product streams is negligible.</p> <p>More information on the Fuel Oils 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 Fuel Oils Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
<p>Conclusion:</p>	<p>Summary</p> <p>In the environment, hydrolysis will not contribute to the degradation of constituent chemicals in the Fuel Oils Category. The Fuel Oils Category includes eight process streams:</p> <ul style="list-style-type: none">• Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit• Light Pyrolysis Fuel Oil from the Ethylene Process Unit• Quench Oil from the Ethylene Process Unit Water Quench System• Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation• Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units• Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Gasoline Units• Hydrotreated Flux Oil• Biphenyl Concentrate <p>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 Fuel Oils Category</u></p> <p>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible. Twelve CAS numbers (see <u>Test Substance</u>) identify products derived from these process streams. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C8-C14. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Fuel Oils</u>.</p>

Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

	<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>More information on the Fuel Oils 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 eight process streams in this category are:</p> <ul style="list-style-type: none">• Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit: In ethylene plants cracking liquid feedstocks, the cracking furnace effluent (after heat recovery) is further quenched by injection of recycled quench oil. This step results in the condensation of higher boiling hydrocarbon compounds that are typically separated from the rest of the furnace effluent as the bottoms of the primary fractionation tower or oil quench tower. Lights are stripped from the excess oils generated from this quench system, resulting in the stream identified here as heavy pyrolysis fuel oil consisting of C10+ and considerable PAHs.• Light Pyrolysis Fuel Oil from the Ethylene Process Unit: In some cases, a light pyrolysis fuel oil is produced from the oil quench system in an ethylene plant that cracks liquid feedstocks. This stream may be produced as a side draw from the primary fractionation tower. The stream typically has a carbon number distribution of C9 to C14 and the major components are naphthalene (30 to 60%), methyl naphthalenes and other substituted one and two ring aromatics.• Quench Oil from the Ethylene Process Unit Water Quench System: In ethylene plants cracking only gases, the cracking furnace effluent (after heat recovery) may be further quenched with water. This step results in the condensation of a relatively small amount of higher boiling hydrocarbon components that, after stripping to remove lights, may be isolated as the Quench Oils from the Ethylene Process Unit Water Quench System. This stream is predominantly C7 through components boiling at 650°F or higher. The reported composition indicates 0.1% benzene, 5% toluene, 12% C8 aromatics, 5% naphthalene, 10% anthracene and 65% C7-C18 cyclic olefins.• Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation: This stream is separated by distillation from pyrolysis gasoline, as a bottoms product. The reported composition indicates a carbon number distribution of from C9 to hydrocarbons boiling at 650°F or higher. The reported typical composition includes 20% dicyclopentadiene, 30% codimers of C5 and C6 monomers, 20% naphthalene and substituted naphthalenes.
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Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

	<ul style="list-style-type: none">• Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units: A single combined fuel oil stream for the ethylene process unit and the pyrolysis gasoline unit is not an uncommon situation for the industry. The carbon number distribution for this stream is generally C10 to compounds with a boiling point of 650°F or higher. At least in some cases, lower carbon number components are reported for the stream, e.g. C5s at approximately 2% and benzene at up to 4%. The major components reported in the stream are typically 25% C9 compounds, 10-47% naphthalene and 4-30% methylnaphthalenes.• Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Gasoline Units: Ethylene process operations that include both a pyrolysis gasoline distillation unit and a benzene hydrodealkylation unit may combine the fuel oil streams from these two units resulting in a single isolated product. Fuel oil is produced in the benzene HDA process by the HDA reactors and separated as a distillation bottoms product. The carbon number distribution for this combined fuel stream is C9 through hydrocarbons with a boiling point of 650°F or higher, although relatively low levels of lower carbon number hydrocarbons may be present, e.g. 0.2% benzene. The major components reported in the stream include 11% C9 aromatics to naphthalene, 7.5-12% DCPD, 7-13% naphthalene, 22% methylnaphthalenes, and 25-35% biphenyl.• Hydrotreated Flux Oil: is a hydrotreated fuel oil stream with a carbon number distribution predominantly C10 to hydrocarbons with a boiling point of 650°F or higher. The stream may be produced as distillation bottoms from a pyrolysis gasoline hydrotreater unit. The components in the stream are predominantly aromatics, paraffins and cyclic compounds. This stream differs from the other fuel oils described above in that its diolefin and vinyl aromatic content is very low.• Biphenyl Concentrate: is a co-product of the benzene hydrodealkylation unit that is isolated by distillation from the HDA reactor effluent. The carbon number distribution for the stream is C7 to C18, with the major component reported to be 65 to 95% biphenyl.
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Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

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. 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.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Fuel Oils 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).

The substances in the Fuel Oils Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Fuel Oils Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Fuel Oils 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.

Hydrolysis (Stability in Water)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1;
68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E067

Reliability:	These data represent a key study for characterizing the potential of substances in the Fuel Oils Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis. Fuel Oils Category. Rosslyn, VA, 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 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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E070

FUEL OILS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E070

<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 Fuel Oils Category</u></p> <p>The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of lower boiling materials. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations.</p> <p>Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C8-C14. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated <u>Fuel Oils</u>.</p> <p>The five chemicals selected to represent the atmospheric oxidation potential of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E070

<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>indene</td> <td>53.0</td> <td>2.4 E⁻¹²</td> </tr> <tr> <td>dicyclopentadiene</td> <td>1.1</td> <td>119.2 E⁻¹²</td> </tr> <tr> <td>naphthalene</td> <td>5.9</td> <td>21.6 E⁻¹²</td> </tr> <tr> <td>methylnaphthalene</td> <td>2.3</td> <td>56.5 E⁻¹²</td> </tr> <tr> <td>1,1'-biphenyl</td> <td>18.9</td> <td>6.8 E⁻¹²</td> </tr> </tbody> </table> <p>* Atmospheric half-life values are based on a 12-hr day.</p> <p>More information on the Fuel Oils 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"> Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. <i>Environ. Toxicol. Chem.</i> 7:435-442. 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. 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. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Fuel Oils 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>	indene	53.0	2.4 E ⁻¹²	dicyclopentadiene	1.1	119.2 E ⁻¹²	naphthalene	5.9	21.6 E ⁻¹²	methylnaphthalene	2.3	56.5 E ⁻¹²	1,1'-biphenyl	18.9	6.8 E ⁻¹²						
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<p>Degradation Products**:</p> <ul style="list-style-type: none"> Note: Identification, concentration 	<p>Unknown</p>																								
<p>Test Substance:</p>	<p>The Fuel Oils Category includes the following CAS numbers:</p> <table border="0"> <tr> <td>64741-62-4</td> <td>Clarified oils, petroleum, catalytic cracked</td> </tr> <tr> <td>64742-90-1</td> <td>Residues, petroleum, steam cracked</td> </tr> <tr> <td>68131-05-5</td> <td>Hydrocarbon oils, process blends</td> </tr> <tr> <td>68409-73-4</td> <td>Aromatic hydrocarbons, biphenyl-rich</td> </tr> <tr> <td>68475-80-9</td> <td>Distillates, petroleum, light steam-cracked naphtha</td> </tr> <tr> <td>68513-69-9</td> <td>Residues, petroleum, steam cracked light</td> </tr> <tr> <td>68514-34-1</td> <td>Hydrocarbons, C9-14, ethylene-manufacture-by-product</td> </tr> <tr> <td>68527-18-4</td> <td>Gas oils, petroleum, steam-cracked</td> </tr> <tr> <td>68921-67-5</td> <td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td> </tr> <tr> <td>69013-21-4</td> <td>Fuel oil, pyrolysis</td> </tr> <tr> <td>69430-33-7</td> <td>Hydrocarbons, C6-30</td> </tr> <tr> <td>8002-05-9</td> <td>Petroleum</td> </tr> </table>	64741-62-4	Clarified oils, petroleum, catalytic cracked	64742-90-1	Residues, petroleum, steam cracked	68131-05-5	Hydrocarbon oils, process blends	68409-73-4	Aromatic hydrocarbons, biphenyl-rich	68475-80-9	Distillates, petroleum, light steam-cracked naphtha	68513-69-9	Residues, petroleum, steam cracked light	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacture-by-product	68527-18-4	Gas oils, petroleum, steam-cracked	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	69013-21-4	Fuel oil, pyrolysis	69430-33-7	Hydrocarbons, C6-30	8002-05-9	Petroleum
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Photodegradation (Indirect)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E070

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 1.1 to 53 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 12 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 Fuel Oils 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.
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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E063

FUEL OILS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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 Fuel Oils Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the log K_{ow} range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers.</p> <p>Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</p>

Partition Coefficient (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E063

<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="695 321 829 380">Substance Constituent</th><th data-bbox="906 321 1089 380">Calculated log K_{ow} @ 25°C</th><th data-bbox="1149 321 1333 380">Measured* log K_{ow} @ 25°C</th></tr></thead><tbody><tr><td data-bbox="695 415 773 436">indene</td><td data-bbox="987 415 1040 436">2.88</td><td data-bbox="1235 415 1268 436">na</td></tr><tr><td data-bbox="695 447 906 468">dicyclopentadiene</td><td data-bbox="987 447 1040 468">3.16</td><td data-bbox="1235 447 1268 468">na</td></tr><tr><td data-bbox="695 478 829 499">naphthalene</td><td data-bbox="987 478 1040 499">3.17</td><td data-bbox="1219 478 1284 499">3.30</td></tr><tr><td data-bbox="695 510 919 531">methylnaphthalene</td><td data-bbox="987 510 1040 531">3.72</td><td data-bbox="1219 510 1284 531">3.86</td></tr><tr><td data-bbox="695 541 846 562">1,1'-biphenyl</td><td data-bbox="987 541 1040 562">3.76</td><td data-bbox="1219 541 1284 562">3.98</td></tr></tbody></table> <p data-bbox="695 594 1414 709">* Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the 12 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated log K _{ow} @ 25°C	Measured* log K _{ow} @ 25°C	indene	2.88	na	dicyclopentadiene	3.16	na	naphthalene	3.17	3.30	methylnaphthalene	3.72	3.86	1,1'-biphenyl	3.76	3.98						
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Partition Coefficient (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E063

Conclusion:	The calculated log K_{ow} for selected representative constituents that are present in category streams range from 2.88 to 3.76 @ 25°C. The measured log K_{ow} of these same constituents range from 3.30 to 3.98 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside of these ranges may be possible for some category streams.
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 log K_{ow} range for substances represented by the 12 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 Fuel Oils 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.
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 10/03)

* 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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E061

FUEL OILS ROBUST SUMMARY**Melting Point**

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: <u>Environmental Exposure from Chemicals</u>. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.</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 Fuel Oils Category are listed below. The data identify a potential melting point range for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the melting point range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</p>

Melting Point (Range)

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Robust Summary No.: OP E061

<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>indene</td> <td>24.36</td> <td>na</td> </tr> <tr> <td>dicyclopentadiene</td> <td>-16.78</td> <td>32.0</td> </tr> <tr> <td>naphthalene</td> <td>5.01</td> <td>80.2</td> </tr> <tr> <td>methylnaphthalene</td> <td>22.15</td> <td>34.4</td> </tr> <tr> <td>1,1'-biphenyl</td> <td>25.07</td> <td>69.0</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential melting point range for substances represented by the 12 CAS numbers under <u>Test Substance</u>.</p>	Substance <u>Constituent</u>	Calculated <u>MP (°C)</u>	Measured* <u>MP (°C)</u>	indene	24.36	na	dicyclopentadiene	-16.78	32.0	naphthalene	5.01	80.2	methylnaphthalene	22.15	34.4	1,1'-biphenyl	25.07	69.0						
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<p>Test Substance:</p>	<p>The Fuel Oils Category includes the following CAS numbers:</p> <table border="1"> <tbody> <tr> <td>64741-62-4</td> <td>Clarified oils, petroleum, catalytic cracked</td> </tr> <tr> <td>64742-90-1</td> <td>Residues, petroleum, steam cracked</td> </tr> <tr> <td>68131-05-5</td> <td>Hydrocarbon oils, process blends</td> </tr> <tr> <td>68409-73-4</td> <td>Aromatic hydrocarbons, biphenyl-rich</td> </tr> <tr> <td>68475-80-9</td> <td>Distillates, petroleum, light steam-cracked naphtha</td> </tr> <tr> <td>68513-69-9</td> <td>Residues, petroleum, steam cracked light</td> </tr> <tr> <td>68514-34-1</td> <td>Hydrocarbons, C9-14, ethylene-manufacture-by-product</td> </tr> <tr> <td>68527-18-4</td> <td>Gas oils, petroleum, steam-cracked</td> </tr> <tr> <td>68921-67-5</td> <td>Hydrocarbons, ethylene-manufacture-by-product distillation residues</td> </tr> <tr> <td>69013-21-4</td> <td>Fuel oil, pyrolysis</td> </tr> <tr> <td>69430-33-7</td> <td>Hydrocarbons, C6-30</td> </tr> <tr> <td>8002-05-9</td> <td>Petroleum</td> </tr> </tbody> </table> <p>The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of lower boiling materials. The 12 CAS numbers are used to describe the eight process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible.</p> <p>More information on the Fuel Oils 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 Fuel Oils Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.</p>	64741-62-4	Clarified oils, petroleum, catalytic cracked	64742-90-1	Residues, petroleum, steam cracked	68131-05-5	Hydrocarbon oils, process blends	68409-73-4	Aromatic hydrocarbons, biphenyl-rich	68475-80-9	Distillates, petroleum, light steam-cracked naphtha	68513-69-9	Residues, petroleum, steam cracked light	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacture-by-product	68527-18-4	Gas oils, petroleum, steam-cracked	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	69013-21-4	Fuel oil, pyrolysis	69430-33-7	Hydrocarbons, C6-30	8002-05-9	Petroleum
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Melting Point (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E061

Conclusion:	The calculated melting points for selected representative constituents that are present in category streams range from -16.78 to 25.07 °C. The measured melting points of these same constituents range from 32.0 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.
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 melting point range for substances represented by the 12 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 Fuel Oils 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.
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 10/03)

* 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.

Vapor Pressure (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E062

FUEL OILS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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 Fuel Oils Category are listed below. The data identify a potential vapor pressure range for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the vapor pressure range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</p>

Vapor Pressure (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E062

<p>Results: (cont'd)</p> <p>Units/Value:</p> <ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	<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>indene</td> <td>0.25</td> <td>na</td> </tr> <tr> <td>dicyclopentadiene</td> <td>2.2</td> <td>3.05</td> </tr> <tr> <td>naphthalene</td> <td>0.11</td> <td>0.05</td> </tr> <tr> <td>methylnaphthalene</td> <td>4.60 E⁻²</td> <td>7.33 E⁻²</td> </tr> <tr> <td>1,1'-biphenyl</td> <td>9.99 E⁻³</td> <td>1.19 E⁻²</td> </tr> </tbody> </table> <p>* Experimental values from EPIWIN database. na = not available</p> <p>The data represent a potential vapor pressure range for substances represented by the 12 CAS numbers under <u>Test Substance</u>.</p>	Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)	indene	0.25	na	dicyclopentadiene	2.2	3.05	naphthalene	0.11	0.05	methylnaphthalene	4.60 E ⁻²	7.33 E ⁻²	1,1'-biphenyl	9.99 E ⁻³	1.19 E ⁻²						
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Vapor Pressure (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E062

Conclusion:	The calculated vapor pressures for selected representative constituents that are present in category streams range from 9.99 E ⁻³ to 2.2 hPa @ 25°C. The measured vapor pressures of these same constituents range from 7.33 E ⁻² to 3.05 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside of these ranges may be possible for some category streams.
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 12 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 Fuel Oils 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 10/03)

* 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.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9
Robust Summary No.: OP E064

FUEL OILS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9]
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 Fuel Oils Category are listed below. The data identify a potential water solubility range for substances represented by the 12 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 complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The five chemicals selected to represent the water solubility range of this category are C9-C12 hydrocarbons that can be found in substances identified by the 12 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category chemistry/structure and olefinic process (distillation) knowledge.</p>

Water Solubility (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E064

<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="691 321 834 384"><u>Substance Constituent</u></th><th data-bbox="914 321 1089 384"><u>Calculated WS (mg/L @ 25°C)</u></th><th data-bbox="1151 321 1326 384"><u>Measured WS* (mg/L @ 25°C)</u></th></tr></thead><tbody><tr><td data-bbox="691 415 776 443">Indene</td><td data-bbox="959 415 1027 443">372.1</td><td data-bbox="1208 415 1243 443">na</td></tr><tr><td data-bbox="691 447 906 474">dicyclopentadiene</td><td data-bbox="967 447 1019 474">51.9</td><td data-bbox="1208 447 1243 474">na</td></tr><tr><td data-bbox="691 478 834 506">naphthalene</td><td data-bbox="959 478 1027 506">183.8</td><td data-bbox="1195 478 1268 506">142.1</td></tr><tr><td data-bbox="691 510 919 537">methylnaphthalene</td><td data-bbox="967 510 1019 537">54.6</td><td data-bbox="1208 510 1268 537">41.4</td></tr><tr><td data-bbox="691 541 841 569">1,1'-biphenyl</td><td data-bbox="967 541 1019 569">44.7</td><td data-bbox="1208 541 1268 569">29.0</td></tr></tbody></table> <p data-bbox="691 600 1425 747">* Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 12 CAS numbers under <u>Test Substance</u>.</p>	<u>Substance Constituent</u>	<u>Calculated WS (mg/L @ 25°C)</u>	<u>Measured WS* (mg/L @ 25°C)</u>	Indene	372.1	na	dicyclopentadiene	51.9	na	naphthalene	183.8	142.1	methylnaphthalene	54.6	41.4	1,1'-biphenyl	44.7	29.0						
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<p>Test Substance:</p>	<p data-bbox="691 800 1406 827">The Fuel Oils Category includes the following CAS numbers:</p> <table border="0"><tr><td data-bbox="691 842 834 869">64741-62-4</td><td data-bbox="857 842 1344 869">Clarified oils, petroleum, catalytic cracked</td></tr><tr><td data-bbox="691 873 834 900">64742-90-1</td><td data-bbox="857 873 1284 900">Residues, petroleum, steam cracked</td></tr><tr><td data-bbox="691 905 834 932">68131-05-5</td><td data-bbox="857 905 1247 932">Hydrocarbon oils, process blends</td></tr><tr><td data-bbox="691 936 834 963">68409-73-4</td><td data-bbox="857 936 1295 963">Aromatic hydrocarbons, biphenyl-rich</td></tr><tr><td data-bbox="691 968 834 995">68475-80-9</td><td data-bbox="857 968 1455 995">Distillates, petroleum, light steam-cracked naphtha</td></tr><tr><td data-bbox="691 999 834 1026">68513-69-9</td><td data-bbox="857 999 1344 1026">Residues, petroleum, steam cracked light</td></tr><tr><td data-bbox="691 1031 834 1058">68514-34-1</td><td data-bbox="857 1031 1425 1083">Hydrocarbons, C9-14, ethylene-manufacture-by-product</td></tr><tr><td data-bbox="691 1087 834 1115">68527-18-4</td><td data-bbox="857 1087 1268 1115">Gas oils, petroleum, steam-cracked</td></tr><tr><td data-bbox="691 1119 834 1146">68921-67-5</td><td data-bbox="857 1119 1430 1171">Hydrocarbons, ethylene-manufacture-by-product distillation residues</td></tr><tr><td data-bbox="691 1176 834 1203">69013-21-4</td><td data-bbox="857 1176 1057 1203">Fuel oil, pyrolysis</td></tr><tr><td data-bbox="691 1207 834 1234">69430-33-7</td><td data-bbox="857 1207 1105 1234">Hydrocarbons, C6-30</td></tr><tr><td data-bbox="691 1239 834 1266">8002-05-9</td><td data-bbox="857 1239 976 1266">Petroleum</td></tr></table> <p data-bbox="691 1304 1471 1577">The Fuel Oils Category was developed by grouping eight ethylene industry streams made up of hydrocarbons that are C8 and higher with varying amounts of lower boiling materials. The 12 CAS numbers are used to describe the eight process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon process streams consisting predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The 1,3-butadiene content of the process streams is negligible.</p> <p data-bbox="691 1608 1430 1692">More information on the Fuel Oils Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).</p> <ol style="list-style-type: none"><li data-bbox="691 1728 1471 1875">1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Fuel Oils Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.	64741-62-4	Clarified oils, petroleum, catalytic cracked	64742-90-1	Residues, petroleum, steam cracked	68131-05-5	Hydrocarbon oils, process blends	68409-73-4	Aromatic hydrocarbons, biphenyl-rich	68475-80-9	Distillates, petroleum, light steam-cracked naphtha	68513-69-9	Residues, petroleum, steam cracked light	68514-34-1	Hydrocarbons, C9-14, ethylene-manufacture-by-product	68527-18-4	Gas oils, petroleum, steam-cracked	68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues	69013-21-4	Fuel oil, pyrolysis	69430-33-7	Hydrocarbons, C6-30	8002-05-9	Petroleum
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Water Solubility (Range)

CAS No.: 64741-62-4; 64742-90-1; 68131-05-5; 68409-73-4; 68475-80-9; 68513-69-9; 68514-34-1; 68527-18-4; 68921-67-5; 69013-21-4; 69430-33-7; 8002-05-9

Robust Summary No.: OP E064

Conclusion:	The calculated water solubility for selected representative constituents that are present in category streams range from 44.7 to 372.1 mg/L @ 25°C. The measured water solubility of these same constituents range from 29.0 to 142.1 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.
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 12 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 Fuel Oils 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.)
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* 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.