Petroleum Distillates (CAS# 64742-94-5) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

ToxServices LLC

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TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING
1367 Connecticut Ave., N.W., Suite 300
Washington, D.C. 20036

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GreenScreen® Executive Summary for Petroleum Distillates (CAS #64742-94-5)

Petroleum distillates, or heavy aromatic solvent naphtha (petroleum), are a class of chemicals that function as degreasing agents, are used in varnishes, lacquers, and synthetic enamels, lithography inks, and textile printing. Additionally, petroleum distillates are used as solvents in herbicides, fungicides, and insecticides.

Petroleum distillates was assigned a GreenScreen® Benchmark Score of 1 ("Avoid – Chemical of High Concern") as it has very High Ecotoxicity (acute aquatic toxicity (AA)), High persistence (P), and very High bioaccumulation (B). This corresponds to GreenScreen® benchmark classification 1a and 1d in CPA 2011. As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), petroleum distillates meets requirements for a GreenScreen® Benchmark Score of 1 without assessing other endpoints. As evaluation of critical endpoints resulted in a Benchmark Score of 1, additional endpoints were not evaluated.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
As a standard approach for GreenScreen® evaluations, all exposure routes (oral, dermal and inhalation) were evaluated together, so the GreenScreen® Benchmark Score of 1 ("Avoid – Chemical of High Concern") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for Petroleum Distillates

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	**M**	**R**	**D**	**E**	**AT**	**ST**		**N**		**SnS***	**SnR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
						single	repeated*	single	repeated*										
N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	**vH**	*H*	*H*	*vH*	N/A	N/A

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms. N/A represents endpoints that were not assessed due to the chemical achieving a Benchmark 1 score following a targeted GreenScreen® analysis.

GreenScreen® Assessment for Petroleum Distillates (CAS #64742-94-5)

Method Version: GreenScreen® Version 1.2[1]
Assessment Type[2]: Certified

Chemical Name: Petroleum distillates

CAS Number: 64742-94-5

GreenScreen® Assessment Prepared By:
Name: Emily Golden, M.F.S.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 14, 2014
Assessor Type: Licensed GreenScreen® Profiler

Quality Control Performed By:
Name: Bingxuan Wang, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 15, 2014

Confirm application of the *de minimus* rule[3]: N/A

Chemical Structure(s):
Unspecified

Also called: (Polyethyl)benzenes; Heavy aromatic naphtha; Heavy aromatic solvent naphtha (petroleum) (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Jet fuel was used as a read-across substance for petroleum distillates in the REACH Dossier for petroleum distillates, as it has a similar range of carbons (i.e., C9-17). Therefore, data on jet fuel were used in the assessment of the persistence endpoint.

Identify Applications/Functional Uses: (Neimeier 2001)
1. Degreasing agent
2. Varnishes, lacquers, and synthetic enamels
3. Lithography inks
4. Textile printing
5. Solvent in herbicides, fungicides, and insecticides

GreenScreen® Summary Rating for Petroleum distillates[4]: Petroleum distillates was assigned a GreenScreen® Benchmark Score of 1 ("Avoid – Chemical of High Concern") as it has Very High Ecotoxicity (acute aquatic toxicity (AA)), High persistence (P), and Very High bioaccumulation (B). This corresponds to GreenScreen® benchmark classification 1a and 1d in CPA 2011. As outlined in

[1] Use GreenScreen® Assessment Procedure (Guidance) V1.2

[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen® Verification Program)

[3] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), petroleum distillates meets requirements for a GreenScreen® Benchmark Score of 1 without assessing other endpoints. As evaluation of critical endpoints resulted in a Benchmark Score of 1, additional endpoints were not evaluated.

Figure 1: GreenScreen® Hazard Ratings for Petroleum Distillates

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	vH	*H*	*H*	*vH*	N/A	N/A

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e. vH, H, M, and L) instead of three (i.e. H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms. N/A represents endpoints that were not assessed due to the chemical achieving a Benchmark 1 score following a targeted GreenScreen® analysis.

Transformation Products and Ratings:

Identify feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

No feasible and relevant transformation products were identified. CO, CO_2, and H_2O may be produced by combustion but are naturally occurring and are not assessed. Hydrolysis is a negligible transformation process as the hydrocarbons do not contain hydrolysable functional groups (U.S. EPA 2001).

Introduction

Petroleum distillates are a complex mixture of various hydrocarbons produced as the result of distillation from aromatic streams. This mixture is primarily composed of aromatic hydrocarbons ranging from 9 to 16 carbons. The boiling range of this mixture is approximately 165°C to 290°C. The vapor pressure of petroleum distillates is relatively high; therefore, this mixture is expected to be volatile (ECHA 2014). These chemicals function as degreasing agents and are used in varnishes, lacquers, and synthetic enamels, lithography inks, and textile printing. Additionally, petroleum distillates are used as solvents in herbicides, fungicides, and insecticides (Niemeier 2001).

ToxServices assessed petroleum distillates against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.69 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It

[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b) and these should be checked separately in conjunction with running the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for petroleum distillates can be found in Appendix C and a summary of the results can be found below:

- Environment Canada – Domestic Substances List (DSL)
  - DSL substances that are Bioaccumulative – GreenScreen® Benchmark Unspecified (LT-U)
- German FEA – Substances Hazardous to Waters (VwVwS)
  - Class 2 Hazard to Water – GreenScreen® Benchmark Possible 1 (LT-P1)
- Environment Canada – Domestic Substances List (DSL)
  - Inherently Toxic to the Environment – GreenScreen® Benchmark Unspecified (LT-U)
- Environment Canada – Domestic Substances List (DSL)
  - Inherently Toxic to Humans: DSL Substances that meet human health categorization criteria – GreenScreen® Benchmark Unspecified (LT-U)

PhysicoChemical Properties of Petroleum distillates

Petroleum distillates are a complex mixture of various hydrocarbons produced as the result of distillation from aromatic streams. This mixture is primarily composed of aromatic hydrocarbons ranging from 9 to 16 carbons. The boiling range of this mixture is approximately 165°C to 290°C. The vapor pressure of petroleum distillates is relatively high; therefore, this mixture is expected to be volatile (ECHA 2014).

Table 1: Physical and Chemical Properties of Petroleum Distillates (CAS #64742-94-5)

Property	Value	Reference
Molecular formula	Unspecified	
SMILES Notation	Unspecified	
Molecular weight	Unspecified	
Physical state	Semi-liquid; semi-solid	ECHA 2014
Appearance	Crystalline and viscous liquid at 20°C and 1013 hPa (760 mm Hg)	ECHA 2014
Melting point	-63°C	ECHA 2014
Vapor pressure	47.89 hPa (35.9 mm Hg) at 20°C	ECHA 2014
Water solubility	41 mg/L at 20°C	ECHA 2014
Dissociation constant	Not Identified	
Density/specific gravity	1.02 g/mL at 20°C	ECHA 2014
Partition coefficient	>3.4 to <5.4	ECHA 2014

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a carcinogen.
  - *Screening:* Petroleum distillates is not listed on any screening lists as a carcinogen.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a mutagen/genotoxicant.
    - *Screening:* Petroleum distillates is not listed on any screening lists as a mutagen/genotoxicant.

Reproductive Toxicity (R) Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a reproductive toxicant.
    - *Screening:* Petroleum distillates is not listed on any screening lists as a reproductive toxicant.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a developmental toxicant.
    - *Screening:* Petroleum distillates is not listed on any screening lists as a developmental toxicant.

Endocrine Activity (E) Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as endocrine active.
    - *Screening:* Petroleum distillates is not listed on any screening lists as endocrine active.
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as an acute toxicant.
    - *Screening:* Petroleum distillates is not listed on any screening lists as an acute toxicant.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)* (vH, H, M, or L): Not Assessed**

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a systemic toxicant (single exposure).
    - *Screening:* Petroleum distillates is not listed on any screening lists as a systemic toxicant

(single exposure).

Group II* Score (repeated dose) **(H, M, or L): Not Assessed**

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a systemic toxicant (repeated exposure).
  - *Screening:* Petroleum distillates is not listed on any screening lists as a systemic toxicant (repeated exposure).

Neurotoxicity (N)

Group II Score (single dose) **(vH, H, M, or L): Not Assessed**

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a neurotoxicant (single exposure).
  - *Screening:* Petroleum distillates is not listed on any screening lists as a neurotoxicant (single exposure).
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

Group II* Score (repeated dose) **(H, M, or L): Not Assessed**

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a neurotoxicant (repeated exposure).
  - *Screening:* Petroleum distillates is not listed on any screening lists as a neurotoxicant (repeated exposure).
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

Skin Sensitization (SnS) Group II* Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a skin sensitizer.
  - *Screening:* Petroleum distillates is not listed on any screening lists as a skin sensitizer.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a respiratory sensitizer.
  - *Screening:* Petroleum distillates is not listed on any screening lists as a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a skin irritant/corrosive chemical.
  - *Screening:* Petroleum distillates is not listed on any screening lists as a skin irritant/corrosive chemical.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as an eye irritant/corrosive chemical.

- *Screening:* Petroleum distillates is not listed on any screening lists as an eye irritant/corrosive chemical.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): vH
Petroleum distillates was assigned a score of Very High for acute aquatic toxicity based on acute aquatic toxicity values ranging from 1 to approximately 3 mg/L. GreenScreen® criteria classify chemicals as a Very High hazard for acute aquatic toxicity when acute aquatic toxicity values are less than or equal to 1 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as an acute aquatic toxicant.
  - *Screening:* Cuprous oxide is listed on the German FEA – Substances Hazardous to Waters (VwVwS) as a "Class 1 Low Hazard to Waters" chemical. This translates to a GreenScreen® Benchmark Unspecified (LT-U).
- ECHA 2014
  - An LC_{50} of 1.0 mg/L was determined in the fish (*Oncorhyncus mykiss*, 96-hr).
  - An EC_{50} of 2.7 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An EC_{50} of 1.2 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An E_rC_{50} of 2 mg/L was determined in green algae (*Pseudokirchnerella subcapitata*, 72-hr).
  - An E_rC_{50} of 1.8 mg/L was determined in green algae (*Pseudokirchnerella subcapitata*, 96-hr).
  - An E_bC_{50} of 1.3 mg/L was determined in green algae (*Pseudokirchnerella subcapitata*, 72-hr).
  - An E_bC_{50} of 1.3 mg/L was determined in green algae (*Pseudokirchnerella subcapitata*, 96-hr).

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *H*
Petroleum distillates was assigned a score of High for chronic aquatic toxicity based on estimated chronic aquatic toxicity values ranging from less than 1 to approximately 3 mg/L. GreenScreen® criteria classify chemicals as a High hazard for chronic aquatic toxicity when the most conservative chronic aquatic toxicity values are between 0.1 and 1 mg/L (CPA 2012a). Confidence was reduced due to lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a chronic aquatic toxicant.
  - *Screening:* Cuprous oxide is listed on the German FEA – Substances Hazardous to Waters (VwVwS) as a "Class 1 Low Hazard to Waters" chemical. This translates to a GreenScreen® Benchmark Unspecified (LT-U).
- U.S. EPA 2012b
  - Modeling was performed using a default structure associated with the CAS number of 64742-94-5 in the ECOSAR database. Petroleum distillates is designated to the neutral organics ECOSAR chemical class. The most conservative predicted ChV values are 1.042 mg/L in fish, 0.782 mg/L in daphnia, and 2.302 mg/L in green algae (Appendix D).

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *H*

Petroleum distillates was assigned a score of High for persistence based on measured and modeled biodegradation half-life estimates ranging from 30 to 126 days. GreenScreen® criteria classify chemicals as a High hazard for persistence when the most conservative half-life of a chemical in soil, its major partitioning compartment, is between 60 and 180 days (CPA 2012a). Confidence was reduced based on the large half-life range and the use of modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a persistent chemical.
  - *Screening:* Cuprous oxide is listed on the German FEA – Substances Hazardous to Waters (VwVwS) as a "Class 1 Low Hazard to Waters" chemical. This translates to a GreenScreen® Benchmark Unspecified (LT-U).
- ECHA 2014
  - The biodegradation of petroleum distillates was evaluated in an OECD Guideline 301D ready biodegradability test. At day 22, 20% biodegradation was achieved for petroleum distillates. After 32 days, petroleum distillates achieved 22% biodegradation. The results of this study indicate that this chemical is not readily biodegradable.
  - An OECD Guideline 301F study was performed to evaluate the biodegradability of petroleum distillates. After 28 days, petroleum distillates achieved 29% biodegradation. The results of this study support the conclusion that petroleum distillates is not readily biodegradable.
  - An OECD Guideline 301F study was performed to evaluate the biodegradability of petroleum distillates. After 28 days, petroleum distillates achieved 7.3% biodegradation. The results of this study support the conclusion that petroleum distillates is not readily biodegradable.
  - The biodegradability of jet fuel was evaluated in soil. This substance was used as a read-across substance for petroleum distillates as it has a similar range of carbons (i.e., C9-17). While this study is not a guideline study, it was considered acceptable for assessment. The half-life of jet fuel ranged from 4.4 to greater than 12 weeks in loam soil, 6.0 to greater than 12 weeks in sand, and 1.7 to greater than 18 weeks in clay. No additional details were provided.
- U.S. EPA 2012a
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that petroleum distillates is not expected to be readily biodegradable. Fugacity modeling predicts 86.6% will partition to soil with a half-life of 75 days, 11.5% will partition to water with a half-life of 38 days, and <1% will partition to sediment with a half-life of 338 days (Appendix E).
- Based on these results, the weight of evidence suggests that the biodegradation of petroleum distillates in its major compartment (i.e., soil) will be between 30 and 126 days based on measured and modeled data. As a result, the persistence of petroleum distillates is expected to be high.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vH*

Petroleum distillates was assigned a score of Very High for bioaccumulation based on being identified as a bioaccumulative chemical on the Canadian DSL list and measured partition coefficient values generally ranging from 3.4 to 5.2. GreenScreen® criteria classify chemicals as a Very High hazard for bioaccumulation when they are identified as bioaccumulative on the Canadian DSL and when partition coefficients are greater than 5 (CPA 2012a). Confidence was reduced because the Canadian DSL is

considered to be a screening list and screening lists are associated with low confidence in hazard scores. Additionally, while the partition coefficients are measured, they span a range of values; therefore, the confidence is low and the most conservative value was selected to be protective.

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a bioaccumulative chemical.
    - *Screening:* Petroleum distillates is listed on the Environment Canada – Domestic Substances List (DSL) as a "DSL substances that are bioaccumulative" chemical. This translates to a GreenScreen® Benchmark Unspecified (LT-U) and a Very High hazard for persistence.
    - *Screening:* Petroleum distillates is listed on the German FEA – Substances Hazardous to Waters (VwVwS) as a "Class 1 Low Hazard to Waters" chemical. This translates to a GreenScreen® Benchmark Unspecified (LT-U).
- ECHA 2014
    - The measured log K_{ow} values range from 3.4 to 5.2.
- ECHA 2014
    - Bioconcentration factors (BCFs) of representative components of the streams in the solvent naphtha (petroleum), heavy aromatics category were estimated to be 39-18,220. The components were not identified and no additional details were provided.
- ESIS 2000
    - In a bioaccumulation assay, fish (*Jordanella floridae*) were exposed to concentrations of 1.0 to 6.8 mg/L of dissolved hydrocarbons. The length of exposure was 128 days. At the end of the study, the fish were killed and analyzed for bioaccumulation of hydrocarbons. The mean bioconcentration factor (BCF) was determined to be 159. No additional details were provided.
    - In a second bioaccumulation assay, fish (*Jordanella floridae*) were exposed to a concentration of 2.54 mg/L of dissolved hydrocarbons. After 112 days of exposure, the fish were killed and analyzed for the presence of hydrocarbons. The bioconcentration factor (BCF) was determined to be 130. No additional details were provided.
    - The bioaccumulation of the water soluble fraction of jet fuel was measured in fish. Rainbow trout eggs were exposed to concentration of dissolved hydrocarbons ranging from 1.4 to 8.0 mg/L. Eggs were hatched by day 4 and the fish were exposed to the test substance through day 112. The fish were killed and tissues analyzed for the presence of hydrocarbons. The mean bioconcentration factor (BCF) was determined to be 88 (±25). No additional details were provided.
    - Although these studies indicate that petroleum distillates are not expected to bioaccumulate, the studies only assessed the bioaccumulation potential of the water soluble fraction. This fraction is not representative of the mixture; therefore, these results are considered to be of low confidence in assessing the bioaccumulation potential of petroleum distillates.
- U.S. EPA 2012a
    - BCFBAF predicts a BCF of 177.2 based on an experimental log K_{ow} of 3.30, indicating this chemical is not likely to bioaccumulate because the BCF is less than 1,000 based on a log K_{ow} of less than 5.
    - While this model indicates that petroleum distillates are not expected to bioaccumulate, the model has only evaluated one chemical of the mixture. This chemical is not representative of the entire mixture; therefore, these results are considered to be of low confidence in assessing the bioaccumulation potential of petroleum distillates.
- Although the bioaccumulation assays performed in fish indicate that petroleum distillates is not expected to be bioaccumulative, the study was performed using only the water soluble fraction of jet

fuel (i.e., dissolved hydrocarbons). As a result, these studies are not representative of the bioaccumulation of petroleum distillates. Further, the EPISuite modeling performed on petroleum distillates (CAS #64742-94-5) is based on one structure of the mixture. Therefore, the EPISuite results on the individual chemical are not considered to be representative of the chemical under review, which is a mixture. Consequently, the most accurate representation of the bioaccumulation potential is based on the measured partition coefficients. These values are supported by the estimated bioconcentration factors on the components of the mixture in addition to the listing of petroleum distillates on the DSL as a bioaccumulative chemical. Therefore, the weight of evidence indicates that petroleum distillates is potentially very bioaccumulative.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a reactive chemical.
    - *Screening:* Petroleum distillates is not listed on any screening lists as a reactive chemical.

Flammability (F) Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
    - *Authoritative:* Petroleum distillates is not listed on any authoritative lists as a flammable chemical.
    - *Screening:* Petroleum distillates is not listed on any screening lists as a flammable chemical.

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APPENDIX A: Hazard Benchmark Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Petroleum Distillates (CAS #64742-94-5)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	**Petroleum distillates**	**64742-94-5**	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	**vH**	*H*	*H*	*vH*	DG	DG

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	Yes	No	No	Yes	No		
2	STOP						
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Petroleum distillates	**1**

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

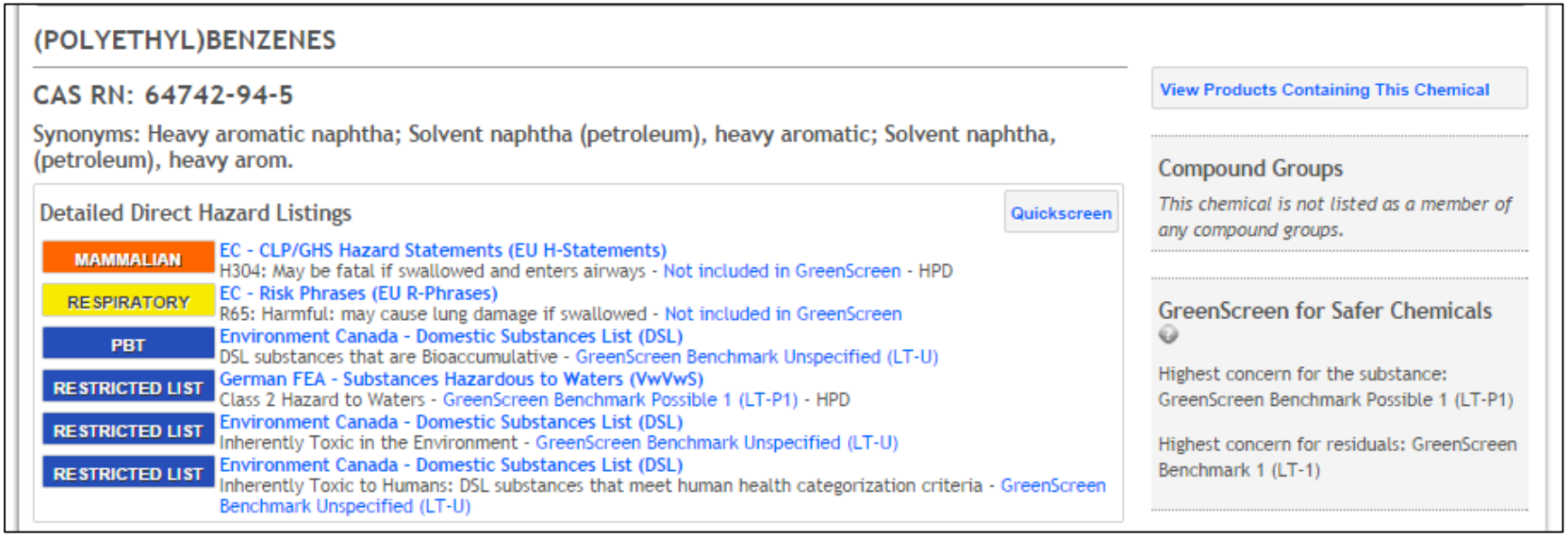
Chemical Name	Final GreenScreen® Benchmark Score
Petroleum distillates	**1**

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												1
2												
3												
4												

APPENDIX C: Pharos Output for Petroleum Distillates (CAS #64742-94-5)



(POLYETHYL)BENZENES

CAS RN: 64742-94-5

Synonyms: Heavy aromatic naphtha; Solvent naphtha (petroleum), heavy aromatic; Solvent naphtha, (petroleum), heavy arom.

Detailed Direct Hazard Listings

Quickscreen

MAMMALIAN — EC - CLP/GHS Hazard Statements (EU H-Statements)
H304: May be fatal if swallowed and enters airways - Not included in GreenScreen - HPD

RESPIRATORY — EC - Risk Phrases (EU R-Phrases)
R65: Harmful: may cause lung damage if swallowed - Not included in GreenScreen

PBT — Environment Canada - Domestic Substances List (DSL)
DSL substances that are Bioaccumulative - GreenScreen Benchmark Unspecified (LT-U)

RESTRICTED LIST — German FEA - Substances Hazardous to Waters (VwVwS)
Class 2 Hazard to Waters - GreenScreen Benchmark Possible 1 (LT-P1) - HPD

RESTRICTED LIST — Environment Canada - Domestic Substances List (DSL)
Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)

RESTRICTED LIST — Environment Canada - Domestic Substances List (DSL)
Inherently Toxic to Humans: DSL substances that meet human health categorization criteria - GreenScreen Benchmark Unspecified (LT-U)

View Products Containing This Chemical

Compound Groups

This chemical is not listed as a member of any compound groups.

GreenScreen for Safer Chemicals

Highest concern for the substance: GreenScreen Benchmark Possible 1 (LT-P1)

Highest concern for residuals: GreenScreen Benchmark 1 (LT-1)

APPENDIX D: ECOSAR Modeling Results for Petroleum Distillates (CAS #64742-94-5)

ECOSAR Version 1.11 Results Page

SMILES: c12ccccc1cccc2
CHEM: Solvent naphtha (petroleum), heavy arom.
CAS Num: 064742-94-5
ChemID1:
MOL FOR: C10 H8
MOL WT: 128.18
Log K_{ow}: 3.169 (EPISuite K_{ow}win v1.68 Estimate)
Log K_{ow}: (User Entered)
Log K_{ow}: 3.30 (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: 80.20 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 52.78 (mg/L, EPISuite WSK_{ow}win v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: 31 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log K_{ow}: 3.169 (EPISuite K_{ow}win v1.68 Estimate)
Wat Sol: 31 (mg/L, PhysProp DB exp value)

Available Measured Data from ECOSAR Training Set

CAS No	Organism	Duration	End Pt	Measured mg/L (ppm)	Ecosar Class	Reference
000091-20-3	Fish	96-hr.	LC50	6.1	Neutral organics	DUL

ECOSAR v1.1 Class-specific Estimations

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr.	LC50	9.387
Neutral Organics	: Daphnid	48-hr.	LC50	5.937
Neutral Organics	: Green Algae	96-hr.	EC50	6.911
Neutral Organics	: Fish		ChV	1.042
Neutral Organics	: Daphnid		ChV	0.782

Neutral Organics	: Green Algae		ChV	2.302
Neutral Organics	: Fish (SW)	96-hr.	LC50	11.900
Neutral Organics	: Mysid	96-hr.	LC50	4.006
Neutral Organics	: Fish (SW)		ChV	2.637
Neutral Organics	: Mysid (SW)		ChV	0.245
Neutral Organics	: Earthworm	14-day	LC50	168.569 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogK_{ow} Cut-Offs

If the log K_{ow} of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogK_{ow}: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogK_{ow}: 6.0 (Earthworm LC50)
Maximum LogK_{ow}: 6.4 (Green Algae EC50)
Maximum LogK_{ow}: 8.0 (ChV)

APPENDIX E: EPISuite Modeling Results for Petroleum Distillates (CAS #64742-94-5)

CAS Number: 64742-94-5
SMILES: c12ccccc1cccc2
CHEM: Solvent naphtha (petroleum), heavy arom.
MOL FOR: C10 H8
MOL WT: 128.18
---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log K_{ow} (octanol-water): ------
Boiling Point (deg C): ------
Melting Point (deg C): ------
Vapor Pressure (mm Hg): ------
Water Solubility (mg/L): ------
Henry LC (atm-m^3/mole): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (K_{ow}WIN v1.68 estimate) = 3.17
Log K_{ow} (Exper. database match) = 3.30
Exper. Ref: HANSCH, C. ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 231.64 (Adapted Stein & Brown method)
Melting Pt (deg C): 5.01 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 0.0404 (Modified Grain method)
VP (Pa, 25 deg C): 5.38 (Modified Grain method)
MP (exp database): 80.2 deg C
BP (exp database): 217.9 deg C
VP (exp database): 8.50E-02 mm Hg (1.13E+001 Pa) at 25 deg C
Subcooled liquid VP: 0.299 mm Hg (25 deg C, exp database VP)
: 39.8 Pa (25 deg C, exp database VP)

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 142.1
log K_{ow} used: 3.30 ($expk_{ow}$ database)
no-melting pt equation used
Water Sol (Exper. database match) = 31 mg/L (25 deg C)
Exper. Ref: PEARLMAN, R.S. ET AL. (1984)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 38.923 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 5.26E-004 atm-m^3/mole (5.33E+001 Pa-m^3/mole)

Group Method: 3.70E-004 atm-m^3/mole (3.75E+001 Pa-m^3/mole)
Exper Database: 4.40E-04 atm-m^3/mole (4.46E+001 Pa-m^3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.795E-005 atm-m^3/mole (4.859E+000 Pa-m^3/mole)
VP: 0.0404 mm Hg (source: MPBPVP)
WS: 142 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 3.30 (exp database)
Log K_{aw} used: -1.745 (exp database)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 5.045
Log K_{oa} (experimental database): 5.190

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 1.0057
Biowin2 (Non-Linear Model): 0.9998
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.3300 (weeks-months)
Biowin4 (Primary Survey Model): 3.3200 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.3966
Biowin6 (MITI Non-Linear Model): 0.4468
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -0.1909
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days): 0.7451
BioHC Half-Life (days): 5.5599

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 39.9 Pa (0.299 mm Hg)
Log K_{oa} (Exp database): 5.190
Kp (particle/gas partition coef. (m^3/ug)):
Mackay model: 7.53E-008
Octanol/air (K_{oa}) model: 3.8E-008
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 2.72E-006
Mackay model: 6.02E-006
Octanol/air (K_{oa}) model: 3.04E-006

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 21.6000 E-12 cm^3/molecule-sec
Half-Life = 0.495 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 5.942 Hrs.
Ozone Reaction:

No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
4.37E-006 (Junge-Pankow, Mackay avg)
3.04E-006 (K_{oa} method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
Koc: 1544 L/kg (MCI method)
Log Koc: 3.189 (MCI method)
Koc: 730.6 L/kg (Kow method)
Log Koc: 2.864 (Kow method)
Experimental Log Koc: 2.96 (database)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 1.844 (BCF = 69.88 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.6560 days (HL = 4.529 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.249 (BCF = 177.2)
Log BAF Arnot-Gobas method (upper trophic) = 2.249 (BAF = 177.4)
log K_{ow} used: 3.30 (expkow database)

Volatilization from Water:
Henry LC: 0.00044 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 2.662 hours
Half-Life from Model Lake: 124 hours (5.165 days)

Removal In Wastewater Treatment:
Total removal: 23.60 percent
Total biodegradation: 0.13 percent
Total sludge adsorption: 8.33 percent
Total to Air: 15.14 percent
(using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment:
Total removal: 44.79 percent
Total biodegradation: 26.30 percent
Total sludge adsorption: 7.26 percent
Total to Air: 11.23 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	0.889	11.9	1000
Water	11.5	900	1000
Soil	86.6	1.8e+003	1000
Sediment	0.998	8.1e+003	0

Persistence Time: 873 hr.

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

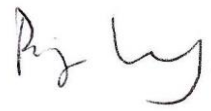
European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

Petroleum Distillates GreenScreen® Evaluation Prepared by:

Emily Golden, M.F.S.
Toxicologist
ToxServices LLC

Petroleum Distillates GreenScreen® Evaluation QC'd by:



Bingxuan Wang, Ph.D.
Toxicologist
ToxServices LLC