Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

State of Washington Department of Ecology

Prepared by:

ToxServices LLC

1367 Connecticut Ave., N.W., Suite 300
Washington, D.C. 20036

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GreenScreen® Executive Summary for Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)

Naphtha (petroleum), hydrotreated light is a chemical that functions as a solvent.

Naphtha (petroleum), hydrotreated light was assigned a GreenScreen® Benchmark Score of LT-1 which may be considered equivalent to a Benchmark 1 ("Avoid-Chemical of High Concern") chemical using the full GreenScreen® method as it has High Group I Human Toxicity (carcinogenicity (C) and mutagenicity (M)). This corresponds to GreenScreen® benchmark classification 1e in CPA 2011.

Under the scope of this project, ToxServices screened all paint components against Clean Production Action's GreenScreen® List Translator (LT). Those identified as List Translator Benchmark 1 chemicals ("LT-1") do not undergo a full GreenScreen® evaluation to save time and resources. Per the scope of work, only those hazard scores driven by authoritative listings in the List Translator search were to be assigned. Upon inspection of the dataset, ToxServices expanded the assessments for all LT-1 chemicals in order to evaluate aquatic toxicity and environmental fate, as these endpoints are highly relevant to the alternatives assessment of nonbiocide boat paints. The expanded environmental fate and toxicity literature search or modeling for Naphtha (petroleum), hydrotreated light did not result in the capture of any additional Benchmark 1 combinations.

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 Naphtha (Petroleum), Hydrotreated Light

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*										
H	**H**	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	**H**	**M**	**vL**	***H***	NA	NA

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. NA: Not assessed.

GreenScreen® Assessment for Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)

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

Chemical Name: Naphtha (petroleum), hydrotreated light

CAS Number: 64742-49-0

GreenScreen® Assessment Prepared By:
Name: Nikki Maples-Reynolds, M.S.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 2, 2014
Assessor Type: Licensed GreenScreen® Profiler

Quality Control Performed By:
Name: Jennifer Rutkiewicz, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 17, 2014

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

Chemical Structure(s):

No structure identified for this complex mixture of hydrocarbons.

Also called: EINECS 265-151-9; Naphtha, petroleum, hydrotreated light; Naphtha (petroleum), hydrotreated light; Naphtha, (petroleum), hydrotreated light; Hydrotreated light straight run (petroleum) (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Naphtha (petroleum), hydrotreated light is a member of OECD's C7-C9 Aliphatic Hydrocarbon Solvents Category (OECD 2010) and ECHA's Low Boiling Point Naphthas (Gasolines) Category (ECHA 2014). Naphtha (petroleum), hydrotreated light has varying compositions of C7 to C9 paraffins with varying compositions of normal paraffins, isoparaffins, and/or cycloparaffins. Category members are compositionally similar refined petroleum derivatives that are expected to have similar toxicological properties based on structural similarity. Data for members of these categories were used in the environmental toxicity and fate assessment.

Identify Applications/Functional Uses:
1. Solvent

GreenScreen® Summary Rating for Naphtha (Petroleum), Hydrotreated Light[4]: Naphtha (petroleum), hydrotreated light was assigned a GreenScreen® Benchmark Score of LT-1 which may be

[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.

considered equivalent to a Benchmark 1 ("Avoid-Chemical of High Concern") chemical using the full GreenScreen® method as it has High Group I Human Toxicity (carcinogenicity (C) and mutagenicity (M)). This corresponds to GreenScreen® benchmark classification 1e in CPA 2011, 2012a. Under the scope of this project, ToxServices screened all paint components against Clean Production Action's GreenScreen® List Translator (LT). Those identified as List Translator Benchmark 1 chemicals ("LT-1") do not undergo a full GreenScreen® evaluation to save time and resources. Per the scope of work, only those hazard scores driven by authoritative listings in the List Translator search were to be assigned. Upon inspection of the dataset, ToxServices expanded the assessments for all LT-1 chemicals in order to evaluate aquatic toxicity and environmental fate, as these endpoints are highly relevant to the alternatives assessment of nonbiocide boat paints. The expanded environmental fate and toxicity literature search or modeling for Naphtha (petroleum), hydrotreated light did not result in the capture of any additional Benchmark 1 combinations.

Figure 1: GreenScreen® Hazard Ratings for Naphtha (Petroleum), Hydrotreated Light

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*										
H	**H**	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	**H**	**M**	**vL**	*H*	NA	NA

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. NA: Not assessed.

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]

Transformation products were not assessed, as naphtha (petroleum), hydrotreated light is an LT-1 chemical and its score will not be impacted by the scores of the transformation products.

Introduction

Naphtha (petroleum), hydrotreated light is a complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C4 through C11 and boiling in the range of approximately minus 20°C to 190°C (-4°F to 374°F) (ECHA 2014).

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

[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.

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 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 naphtha (petroleum), hydrotreated light can be found in Appendix C and a summary of the results can be found below:

- Carcinogenicity
  - EC REACH Annex XVII (EU CMR(1)) Category 2 Carcinogen
  - EU Risk Phrase R45 – may cause cancer
  - GHS Hazard Statement H350 – may cause cancer
  - EC CLP Inventory (EU CMR(2)) Category 1 B Carcinogen
- Gene mutation
  - EU Risk Phrase R46 – may cause heritable genetic damage
  - GHS Hazard Statement H340 – may cause genetic defects
  - EC CLP Inventory (EU CMR(2)) Category 1 B Mutagen
- Mammalian
  - GHS Hazard Statement H304 – may be fatal if swallowed and enters airway
  - EU Risk Phrase R65 – Harmful: may cause lung damage if swallowed
- PBT
  - Canada – DSL – substances that are persistent
- Restricted List
  - ChemSec – Substitution List – Classified CMR (Carcinogen, Mutagen &/or Reproductive Toxicant)
  - German FEA – (VwVwS) Class 3 Severe Hazard to water
  - Environment Canada – DSL inherently toxic to humans
  - Environment Canada – DSL inherently toxic to environment

PhysicoChemical Properties of Naphtha (Petroleum), Hydrotreated Light

Naphtha (petroleum), hydrotreated light is a liquid petroleum mixture under standard temperature and pressure. It has a vapor pressure of 4-240 hPa indicating that it will likely exist in the vapor and liquid phases. It has a log K_{ow} estimated to be >3, indicating that it is more soluble in octanol than in water and that it has the potential to bioaccumulate in aquatic biota.

Table 1: Physical and Chemical Properties of Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)

Property	Value	Reference
Molecular formula	Mixture - variable	
SMILES Notation	Mixture - variable	
Molecular weight	Mixture - variable	
Physical state	Liquid[6]	ECHA 2014
Appearance	Colorless low viscosity, mobile	ECHA 2014

[6] Read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas

Table 1: Physical and Chemical Properties of Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)		
Property	**Value**	**Reference**
	liquid[7]	
Melting point	< -60°C[8]	ECHA 2014
Vapor pressure	4-240 KPa at 37.8°C [9]	ECHA 2014
Water solubility	Not identified	
Dissociation constant	Not identified	
Density/specific gravity	0.62 - 0.88 at 15ºC [10]	ECHA 2014
Partition coefficient	Log K_{ow} > 3[11]	ECHA 2014

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): H
Naphtha (petroleum), hydrotreated light was assigned a score of High for carcinogenicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a High hazard for carcinogenicity when the chemical is listed on the EU CMR (1 or 2) lists or is associated with R45 or H350 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC REACH Annex XVII (EU CMR(1)) Category 2 Carcinogen
  - *Authoritative:* EU Risk Phrase R45 – may cause cancer
  - *Authoritative:* GHS Hazard Statement H350 – may cause cancer
  - *Authoritative:* EC CLP Inventory (EU CMR(2)) Category 1 B Carcinogen
  - *Screening:* Not present on any screening lists

Mutagenicity/Genotoxicity (M) Score (H, M, or L): H
Naphtha (petroleum), hydrotreated light was assigned a score of High for mutagenicity/genotoxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a High hazard for mutagenicity/genotoxicity when the chemical is listed on the EU CMR (1) (Category 2) or (2) (Mutagen 1B) or is associated with R46 or H340 (CPA 2012a).

  - *Authoritative:* EU Risk Phrase R46 – may cause heritable genetic damage
  - *Authoritative:* GHS Hazard Statement H340 – may cause genetic defects
  - *Authoritative:* EC CLP Inventory (EU CMR(2)) Category 1 B Mutagen
  - *Screening:* Not present on any screening lists

[7] Read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas
[8] Gasoline (motor and aviation gasoline) has a melting point of < -60°C (read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas)
[9] The vapor pressures of Low Boiling Point Naphthas (Gasolines) are specified in the range from 4-240 KPa at 37.8°C as measured by EN 13016-1 (read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas)
[10] The density of low boiling point (gasoline) naphthas as measured by EN ISO 12185 lies in the 0.62 - 0.88 range at 15ºC (read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas)
[11] Most of the hydrocarbon blocks comprising gasoline have a Log Kow > 3, indicating these constituents have a potential to bioaccumulate. However, biotransformation is expected to play an important mitigating role in limiting actual bioaccumulation, particularly in higher organisms that possess extensive enzymatic capabilities to metabolize hydrocarbons. However, this endpoint has been calculated for representative hydrocarbon structures using the BCFWIN v2.16 model within EPISuite 3.12 as input to the hydrocarbon block method incorporated into the PETRORISK model (ECHA 2014).

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): H

Naphtha (petroleum), hydrotreated light was assigned a score of High for acute aquatic toxicity based on acute aquatic toxicity values ranging from 3.1 to 64 mg/L. GreenScreen® criteria classify chemicals as a High hazard for acute aquatic toxicity when the most conservative acute aquatic toxicity values fall between 1 and 10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Environment Canada – DSL inherently toxic to environment
- OECD 2014
  - Classification as inherently toxic on the DSL is based on modeled data. The pivotal value used for the conclusion was 0.05 mg/L.
- ECHA 2014

  Note: Data presented below are for members of the Low Boiling Point Naphthas (Gasolines) that were identified as read across chemicals in the REACH dossier.
  - An LL_{50} of 8.2 mg/L was determined in the fish (*Pimephales promelas*, 96-hr).
  - An LL_{50} of 10 mg/L was determined in the fish (*Pimephales promelas*, 96-hr).
  - An LL_{50} of 11 mg/L was determined in the fish (*Pimephales promelas*, 96-hr).
  - An EL_{50} of 4.5 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An EL_{50} of 12 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An EL_{50} of 8.4 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An EL_{50} of 3.1 mg/L was determined in algae (*Selenastrum capricornutum*, 72-hr).
  - An EL_{50} of 3.7 mg/L was determined in algae (*Selenastrum capricornutum*, 96-hr).
  - An EC_{50} of 64 mg/L was determined in algae (*Selenastrum capricornutum*, 96-hr).
  - An EL_{50} of 6.4 mg/L was determined in algae (*Selenastrum capricornutum*, 96-hr).

- OECD 2010

  Multi-constituent members of OECD's C7-C9 Aliphatic Hydrocarbon Solvents Category have measured LC/EC_{50} values from 0.3-1.3 mg/L in fish (96-h), 0.7-0.9 mg/L in daphnia (48-h), and 0.4 mg/L in algae (72-h). The corresponding LL/EL_{50} values were not provided.
- Since classification on the DSL was based on modeled data, this classification on the screening list was disregarded in favor of measured data. While the acute aquatic toxicity values for low boiling point naphthas ranged from 3.1 to 64 mg/L, the weight of evidence suggests that the acute aquatic toxicity values tend to range between 1 and 10 mg/L, indicating that naphtha (petroleum), hydrotreated light is associated with a High hazard for acute aquatic toxicity. Only LC/EC_{50} values were provided for OECD's multi-constituent members of OECD's C7-C9 Aliphatic Hydrocarbon Solvents Category. Naphtha (petroleum), hydrotreated light is a complex mixture of compounds, with solubility of each varying from negligible to slight (OECD 2010). The use of LL/EL_{50} values rather than LC/EC_{50} values is more appropriate for complex substances with a wide range of water solubilities (UN 2013). Therefore the score of High was assigned based on numerous LL/EL_{50} values of compositionally similar compounds.

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): M

Naphtha (petroleum), hydrotreated light was assigned a score of Moderate for chronic aquatic toxicity based on measured and modeled chronic aquatic toxicity values ranging from 0.2 to 20.7 mg/L. GreenScreen® criteria classify chemicals as a Moderate hazard for chronic aquatic toxicity when the most conservative chronic aquatic toxicity values fall between 1 and 10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Environment Canada – DSL inherently toxic to environment
- OECD 2014
  - Classification as inherently toxic on the DSL is based on modeled data. The pivotal value used for the conclusion was 0.05 mg/L.
- ECHA 2014

  Note: Data presented below are for members of the Low Boiling Point Naphthas (Gasolines) that were identified as read across chemicals in the REACH dossier.
  - A NOELR of 2.6 mg/L was determined in the fish for mortality (*Pimephales promelas*, 14-d).
  - An LL_{50} of 5.2 mg/L was determined in the fish (*Pimpehales promelas*, 14-d).
  - A NOELR of 2.6 mg/L was determined in the aquatic invertebrate for reproduction (*Dapnia magna*, 21-d).
  - An EL_{50} of 10 mg/L was determined in the aquatic invertebrate for reproduction (*Daphnia magna*, 21-d).
  - A NOELR of 16 mg/L was determined in the aquatic invertebrate for mortality (*Daphnia magna*, 21-d).
  - An EL_{50} of >40 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 21-d).
  - A NOELR of 6.3 mg/L was determined in the aquatic invertebrate for reproduction (*Daphnia magna*, 21-d).
  - A NOELR of 16 mg/L was determined in the aquatic invertebrate for mortality (*Daphnia magna*, 21-d).
  - An EL_{50} of 13 mg/L was determined in the aquatic invertebrate for reproduction (*Daphnia magna*, 21-d).
  - An EL_{50} of 27 mg/L was determined in the aquatic invertebrate for mortality (*Daphnia magna*, 21-d).

  - A NOELR of 0.5 mg/L was determined in algae for growth rate (*Selenastrum capricornutum*, 72-hr).
  - A NOELR of 51 mg/L was determined in algae for cell density (*Selenastrum capricornutum*, 96-hr).
  - A NOELR of 1.9 mg/L was determined in algae for cell density (*Selenastrum capricornutum*, 96-hr).
  - A NOELR of 10 mg/L was determined in algae for growth rate (*Selenastrum capricornutum*, 72-hr).
- OECD 2010
  - A multi-constituent member of OECD's C7-C9 Aliphatic Hydrocarbon Solvents Category (not specified) has a 21-day NOELR of 1.0 mg/L (NOEC of 0.17 mg/L) in daphnia based on reproduction.
- U.S. EPA 2012b
  - Naphtha (petroleum), hydrotreated light is designated to the neutral organics ECOSAR chemical class. The most conservative predicted ChV values are 0.247 mg/L in fish, 0.214 mg/L in daphnia, and 0.771 mg/L in green algae (Appendix D).
- Since classification on the DSL was based on modeled data, this classification on the screening list was disregarded in favor of measured data. While the chronic aquatic toxicity values for low boiling point naphthas ranged from 0.5 to 51 mg/L, the weight of evidence suggests that the chronic aquatic toxicity values tend to range between 1 and 10 mg/L, indicating that light aliphatic petroleum naphtha is associated with a Moderate hazard for chronic aquatic toxicity.

Environmental Fate (Fate)

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

Naphtha (petroleum), hydrotreated light was assigned a score of Very Low for persistence as the chemical was classified as readily biodegradable. GreenScreen® criteria classify chemicals as Very Low for persistence when they are determined to be readily biodegradable and the dominant compartment is water (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Environmental Canada – DSL substances that are persistent
- ECHA 2014
  - An OECD Guideline 301F ready biodegradability test was performed to assess the biodegradability of light aliphatic petroleum naphtha. The test substance achieved 77% biodegradation in 28 days. Additionally, the authors stated that the test substance met the criteria for ready biodegradability.
  - Light aliphatic petroleum naphtha had a measured biodegradation rate of 94% in 25 days. No details were provided on the ready biodegradability of the substance, and the authors categorized light aliphatic petroleum naphtha as "inherently biodegradable".
  - Light aliphatic petroleum naphtha achieved 74% biodegradation in 28 days. The authors categorized the test substance as "inherently biodegradable". No additional details were provided.
- OECD 2010
  - Multi-constituent members of OECD's C7-C9 Aliphatic Hydrocarbon Solvents Category are expected to be readily biodegradable. OECD reports that multi-constituent members demonstrate > 60% degradation after 28 days but do not meet the 10-day window in tests according to OECD Guideline 301F.

- U.S. EPA 2012a
    - The BIOWIN modeling Ready Biodegradable Predictor indicates that naphtha (petroleum), hydrotreated light is expected to be readily biodegradable. Fugacity modeling predicts 63.4% will partition to water with a half-life of 9 days, 34.9% will partition to air with a half-life of 1.5 days, 1.19% will partition to soil with a half-life of 17 days, and <1% will partition to sediment with a half-life of 78 days (Appendix E).
- In general, measured biodegradation data indicate that naphtha (petroleum), hydrotreated light is expected to be readily biodegradable. This is supported by two studies that, although not ready biodegradability studies, illustrate that the chemical will biodegrade quickly, and OECD's report that multi-constituent category members are expected to be readily biodegradable. Further, biodegradation modeling supports that this chemical will be readily biodegradable. Although the chemical is listed on the DSL as a persistent chemical, no details are available regarding this classification (OECD 2014) and the weight of evidence indicates that this chemical will not be persistent in its dominant compartment (water).

Bioaccumulation (B) Score (vH, H, M, L, or vL): *H*
Naphtha (petroleum), hydrotreated light was assigned a score of High for bioaccumulation based on an estimated partition coefficient of 4.66. GreenScreen® criteria classify chemicals as a High hazard for bioaccumulation when the partition coefficient is between 4.5 and 5 and BCF values are between 1,000 and 5,000 (CPA 2012a). Confidence was reduced due to lack of measured data for this complex mixture.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists
- OECD 2010
    - C7-C9 Aliphatic Hydrocarbon Solvents Category have low to moderate potential for bioaccumulation based on an experimental BCF of 199 in mussels for one category member (n-octane) and modeled BCF values of 105-1,216 for constituents.
- U.S. EPA 2012a
    - BCFBAF predicts a BCF of 682 based on a measured log K_{ow} of 4.66 (Appendix E).
- Modeling predicts a BAF of 682 for the naphtha (petroleum), hydrotreated light mixture, but the structure modeled may not represent the chemical components that have the highest bioaccumulation potential. Therefore, a conservative score of High was assigned for this endpoint based on the estimated log K_{ow} of 4.66 and the highest estimated BCF of 1,216 for constituents.

<u>Physical Hazards (Physical)</u>

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

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

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Not present on any screening lists

References

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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 Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)

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	**naptha (petroleum), hydrotreated light**	**64742-49-0**	H	H	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	**H**	**M**	**vL**	*H*	DG	DG

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
naptha (petroleum), hydrotreated light	1

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

Table 6

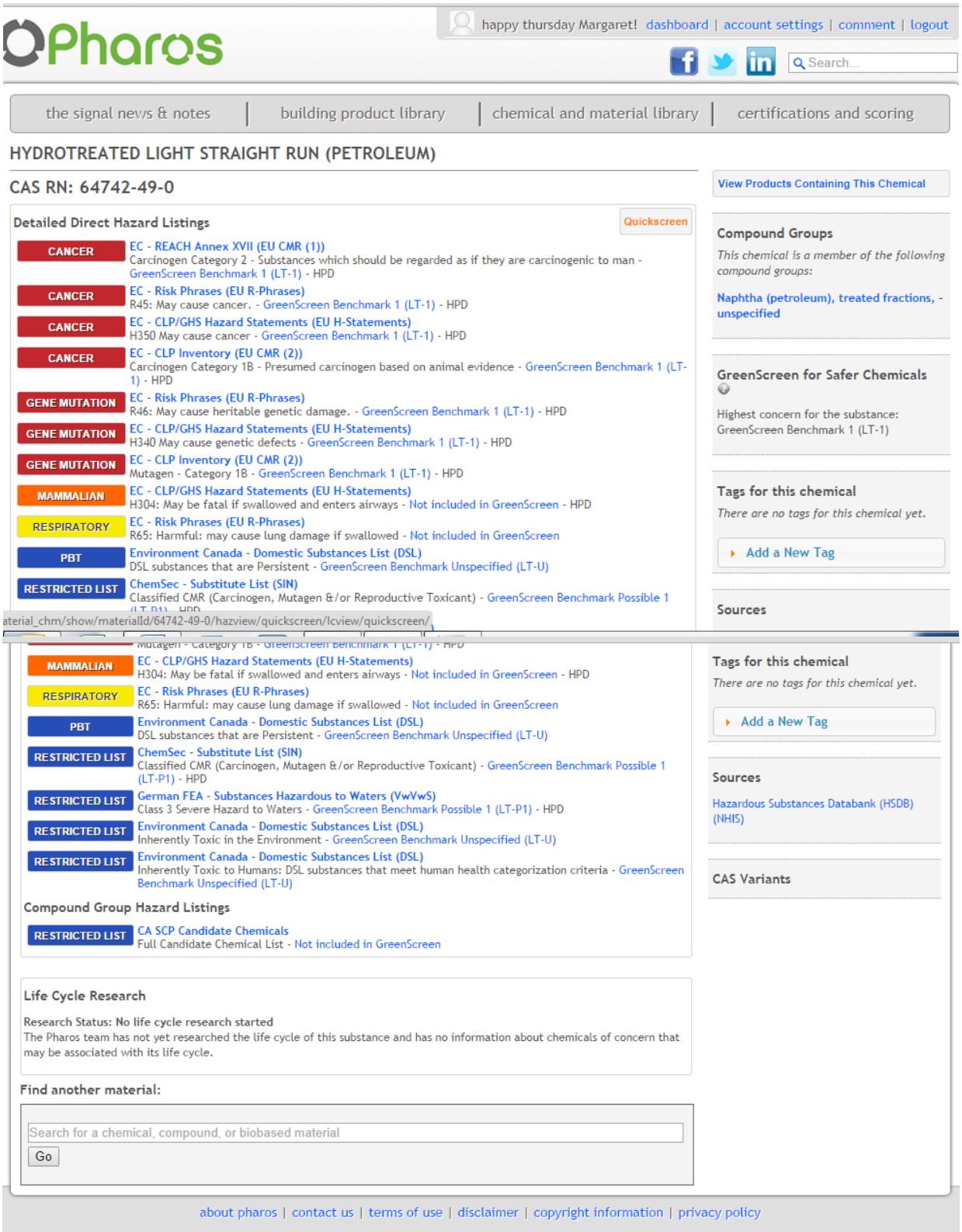
Chemical Name	Final GreenScreen® Benchmark Score
naptha (petroleum), hydrotreated light	1

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 Naphtha (Petroleum), Hydrotreated Light (CAS# 64742-49-0)



APPENDIX D: ECOSAR Modeling Results for Naphtha (Petroleum), Hydrotreated Light (CAS #64742-49-0)

ECOSAR Version 1.11 Results Page

SMILES : CCCCCCC
CHEM: Naphtha (petroleum), hydrotreated light
CAS Num: 064742-49-0
ChemID1:
MOL FOR: C7 H16
MOL WT : 100.21
Log K_{ow}: 3.779 (EPISuite K_{ow}win v1.68 Estimate)
Log K_{ow}: (User Entered)
Log K_{ow}: 4.66 (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: -90.60 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 2.915 (mg/L, EPISuite WSK_{ow}win v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: 3.4 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log K_{ow}: 3.779 (EPISuite K_{ow}win v1.68 Estimate)
Wat Sol: 3.4 (mg/L, PhysProp DB exp value)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr.	LC50	2.078
Neutral Organics	: Daphnid	48-hr.	LC50	1.391
Neutral Organics	: Green Algae	96-hr.	EC50	2.043
Neutral Organics	: Fish		ChV	0.247
Neutral Organics	: Daphnid		ChV	0.214
Neutral Organics	: Green Algae		ChV	0.771

Neutral Organics	: Fish (SW)	96-hr.	LC50	2.644
Neutral Organics	: Mysid	96-hr.	LC50	0.589
Neutral Organics	: Fish (SW)		ChV	0.851
Neutral Organics	: Mysid (SW)		ChV	0.030
Neutral Organics	: Earthworm	14-day	LC50	113.920 *

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 Naphtha (Petroleum), Hydrotreated Light (CAS #64742-49-0)

CAS Number: 64742-49-0
SMILES: CCCCCCC
CHEM: Naphtha (petroleum), hydrotreated light
MOL FOR: C7 H16
MOL WT: 100.21
---------- 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) = 3.78
Log K_{ow} (Exper. database match) = 4.66
Exper. Ref: MILLER, M.M. ET AL. (1985)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 96.16 (Adapted Stein & Brown method)
Melting Pt (deg C): -81.01 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 45.9 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C): 6.12E+003 (Mean VP of Antoine & Grain methods)
MP (exp database): -90.6 deg C
BP (exp database): 98.5 deg C
VP (exp database):4.60E+01 mm Hg (6.13E+003 Pa) at 25 deg C

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 3.554
log K_{ow} used: 4.66 (expK_{ow} database)
no-melting pt equation used
Water Sol (Exper. database match) = 3.4 mg/L (25 deg C)
Exper. Ref: YALKOWSKY, S.H. & DANNENFELSER, R.M. (1992)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 2.6374 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 2.27E+000 atm-m^3/mole (2.30E+005 Pa-m^3/mole)
Group Method: 2.39E+000 atm-m^3/mole (2.42E+005 Pa-m^3/mole)

Exper Database: 2.00E+00 atm-m^3/mole (2.03E+005 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: 1.703E+000 atm-m^3/mole (1.725E+005 Pa-m^3/mole)
VP: 45.9 mm Hg (source: MPBPVP)
WS: 3.55 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 4.66 (exp database)
Log K_{aw} used: 1.913 (exp database)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 2.747
Log K_{oa} (experimental database): 2.950

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.8083
Biowin2 (Non-Linear Model): 0.9686
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.2761 (days-weeks)
Biowin4 (Primary Survey Model): 3.9722 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.6619
Biowin6 (MITI Non-Linear Model): 0.8605
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.4892
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days): 0.7385
BioHC Half-Life (days): 5.4758

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 6.13E+003 Pa (46 mm Hg)
Log K_{oa} (Exp database): 2.950
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model: 4.89E-010
Octanol/air (K_{oa}) model: 2.19E-010
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 1.77E-008
Mackay model: 3.91E-008
Octanol/air (K_{oa}) model: 1.75E-008

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 6.8713 E-12 cm^3/molecule-sec
Half-Life = 1.557 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 18.679 Hrs.
Ozone Reaction:
No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):
2.84E-008 (Junge-Pankow, Mackay avg)
1.75E-008 (K_{oa} method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
K_{oc}: 239.7 L/kg (MCI method)
Log K_{oc}: 2.380 (MCI method)
K_{oc}: 1.107E+004 L/kg (K_{ow} method)
Log K_{oc}: 4.044 (K_{ow} method)

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 = 2.742 (BCF = 551.7 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.2835 days (HL = 1.921 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.834 (BCF = 681.8)
Log BAF Arnot-Gobas method (upper trophic) = 2.837 (BAF = 687.7)
log K_{ow} used: 4.66 (expkow database)

Volatilization from Water:
Henry LC: 2 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 1.022 hours
Half-Life from Model Lake: 95.09 hours (3.962 days)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 99.91 percent
Total biodegradation: 0.12 percent
Total sludge adsorption: 38.71 percent
Total to Air: 61.08 percent
(using 10000 hr. Bio P,A,S)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 99.97 percent
Total biodegradation: 58.86 percent
Total sludge adsorption: 17.68 percent
Total to Air: 23.44 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	34.9	35.9	1000
Water	63.4	208	1000
Soil	1.19	416	1000
Sediment	0.553	1.87e+003	0

Persistence Time: 77 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

Naphtha (petroleum), hydrotreated light GreenScreen® Evaluation Prepared by:

Nikki Maples-Reynolds, MS.
Toxicologist
ToxServices LLC

Naphtha (petroleum), hydrotreated light GreenScreen® Evaluation QC'd by:

Jennifer Rutkiewicz, Ph.D.
Toxicologist
ToxServices LLC