Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

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GreenScreen® Executive Summary for Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6)

Aromatic 100 (Aromatic naphtha, type 1) is a chemical that functions as a solvent for sealants, cleaning, and paints.

Aromatic 100 (Aromatic naphtha, type 1) 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 a 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 Aromatic 100 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 Aromatic 100 (Aromatic naphtha, type 1)

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	L	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 Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6)

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

Chemical Name: Aromatic 100 (Aromatic naphtha, type 1)

CAS Number: 64742-95-6

GreenScreen® Assessment Prepared By:
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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: Aromatic naphtha, type I; Enerade ED-6202; High flash aromatic naphtha; Light aromatic solvent naphtha (petroleum); Petroleum naphtha; High-flash aromatic naphtha, type 1; Solvent naphtha (petroleum), light aromatic, EINECS 265-199-0 (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Aromatic 100 (Aromatic naphtha, type 1) is a member of OECD's C9 Aromatic Hydrocarbon Solvents Category and ECHA's Low Boiling Point Naphthas (Gasolines) Category (ECHA 2014). 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 for varnishing or sealing wood/furniture
2. Solvent for automotive brake and rotor cleaning
3. Solvent for fuel oil tank cleaning
4. Solvent for painting

GreenScreen® Summary Rating for Aromatic 100 (Aromatic naphtha, type 1)[4]: Aromatic 100 (Aromatic naphtha, type 1) 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

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 a 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 aromatic 100 did not result in the capture of any additional Benchmark 1 combinations.

Figure 1: GreenScreen® Hazard Ratings for Aromatic 100 (Aromatic Naphtha, type 1)

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	L	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 Aromatic 100 (Aromatic naphtha, type 1) is an LT-1 chemical and its score will not be impacted by those of transformation products.

Introduction

Aromatic 100 (Aromatic naphtha, type 1) is a complex combination of hydrocarbons obtained from distillation of aromatic streams. It consists predominantly of aromatic hydrocarbons having carbon numbers predominantly in the range of C8 through C10 and boiling in the range of approximately 135°C to 210°C (275°F to 410°F) (ECHA 2014). Aromatic 100 (Aromatic naphtha, type 1) is a solvent for varnishing or sealing wood/furniture, automotive brake and rotor cleaning, fuel oil tank cleaning, and painting (ECHA 2014).

[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.

[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.

ToxServices assessed Aromatic 100 (Aromatic naphtha, type 1) 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 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 Aromatic 100 (Aromatic naphtha, type 1) 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
  - EC - Risk Phrases (EU R-Phrases) R65: Harmful: may cause lung damage if swallowed
  - Canadian – WHMIS Class D2B – Toxic material causing other toxic effects
  - GHS-Japan – Category 4 – Acute toxicity (inhalation: vapors)
  - GHS-Japan – Category 3 – Specific target organs/systemic toxicity following single exposure
  - GHS-Japan – Category 1 – Aspirational hazard
- Skin irritation
  - GHS-Japan – Category 2 – Skin corrosion/irritation
- Flammability
  - GHS-Japan – Category 1 – flammable liquid
  - Québec CSST - WHMIS Classifications (WHMIS) Class B3 - Combustible liquids
- Restricted List
  - ChemSec – Substitution List – Classified CMR (Carcinogen, Mutagen &/or Reproductive Toxicant)
  - German FEA – (VwVwS) Class 2 Hazard to water
  - Environment Canada – DSL inherently toxic to humans

PhysicoChemical Properties of Aromatic 100 (Aromatic naphtha, type 1)

Aromatic 100 (Aromatic naphtha, type 1) 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 Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6)		
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 liquid[7]	ECHA 2014
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 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
Aromatic 100 (Aromatic naphtha, type 1) 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) (Category 2) or (2)(Mutagen 1B) 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
Aromatic 100 (Aromatic naphtha, type 1) 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 or 2) lists or is associated with

[6] Read across from Gasoline - Representative substance for the category of low Boiling Point Naphthas
[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 K_{ow} > 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).

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

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:* Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (inhalation: vapor) - Category 4

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:* Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 3

***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:* Japan METI/MOE - GHS Classifications (GHS-Japan) Skin corrosion/irritation-Category 2

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
Aromatic 100 was assigned a score of High for acute aquatic toxicity as acute aquatic toxicity values ranged 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 are between 1 and 10 mg/L (CPA 2012a).
- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- ECHA 2014
  Note: Data presented 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 (*Oncorhynchus mykiss*, 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 18 mg/L was determined in the aquatic invertebrate (*Daphnia magna*, 48-hr).
  - An EL_{50} of 32 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).
- OECD 2014
  - Aromatic 100 (CAS# 64742-95-6) has a 72-h EC_{50} of 2.4 mg/L (biomass) and 2.7 mg/L (growth) in algae (species not specified).
  - C9 Aromatic Hydrocarbon Solvents category members have LL/EL_{50} and LC/EC_{50} values ranging from 3.5 to 9.2 mg/L in fish and invertebrates based on 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 aromatic 100 is associated with a High hazard for acute aquatic toxicity.

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

Aromatic 100 was assigned a score of Moderate for chronic aquatic toxicity based on the weight of evidence suggesting that the chronic aquatic toxicity values for aromatic 100 are generally between 1 and 10 mg/L. GreenScreen® criteria classify chemicals as a Moderate hazard for chronic aquatic toxicity when chronic aquatic toxicity values range between 1 and 10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- ECHA 2014
  Note: Data presented are for members of the Low Boiling Point Naphthas (Gasolines) that were identified as read across chemicals in the REACH dossier.
  - An NOELR of 2.6 mg/L was determined in the fish for reproduction (*Pimephales promelas*, 14-d).
  - An NOELR of 2.6 mg/L was determined in the aquatic invertebrate for reproduction (*Daphnia magna*, 21-d).
  - An NOELR of 16 mg/L was determined in the aquatic invertebrate for mortality (*Daphnia magna*, 21-d).
  - An NOELR of 6.3 mg/L was determined in the aquatic invertebrate for reproduction (*Daphnia magna*, 21-d).
  - An NOELR of 16 mg/L was determined in the aquatic invertebrate for mortality (*Daphnia magna*, 21-d).
  - An NOELR of 0.5 mg/L was determined in algae for growth rate (*Selenastrum capricornutum*, 72-hr).
  - An NOELR of 51 mg/L was determined in algae for cell density (*Selenastrum capricornutum*, 96-hr).
  - An NOELR of 1.9 mg/L was determined in algae for cell density (*Selenastrum capricornutum*, 96-hr).
  - An NOELR of 10 mg/L was determined in algae for growth rate (*Selenastrum capricornutum*, 72-hr).
- OECD 2012
  - Aromatic 100 (CAS# 64742-95-6) has a 72-h NOEC of 1.3 mg/L (biomass and growth) in algae (species not specified)

- 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 aromatic 100 is associated with a moderate hazard for chronic aquatic toxicity.

Environmental Fate (Fate)

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

Aromatic 100 was assigned a score of very Low for persistence as the chemical was classified as readily biodegradable. GreenScreen® criteria classify chemicals as a very Low hazard for persistence when they are determined to be readily biodegradable when the dominant compartment is soil (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- ECHA 2014
  - The biodegradation of aromatic 100 was assessed in an OECD Guideline 301F ready biodegradability study. After 28 days, 77% biodegradation was achieved. Additionally, the test substance achieved 60% biodegradation within 10 days of achieving 10% biodegradation; therefore, the test substance was considered to be readily biodegradable.
  - Aromatic 100 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 aromatic 100 as "inherently biodegradable".
- OECD 2012
  - C9 Aromatic Hydrocarbon Solvents category members are readily biodegradable.
- U.S. EPA 2012
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that aromatic 100 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 D).
- Measured biodegradation data indicate that light aliphatic petroleum naphtha is expected to be readily biodegradable. This is supported by a study that, although it is not a ready biodegradability study, illustrates that the chemical will biodegrade quickly. Biodegradation modeling indicates that this chemical may not be readily biodegradable; however, the measured ready biodegradability data, in addition to the fact that this chemical has not been flagged on any lists as a persistent chemical, support the conclusion that this chemical will not be persistent in its dominant compartment (soil).

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

Aromatic 100 was assigned a score of Low for bioaccumulation as it has a measured log K_{ow} of 3.3 and an estimated bioconcentration factor (BCF) of 177, and structurally similar C9 Aromatic Hydrocarbon Solvents have measured BCF values of 23-342. GreenScreen® criteria classify chemicals as a Low hazard for bioaccumulation when the BCF is between 100 and 500 or the log K_{ow} is less than 4(CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Not present on any screening lists
- OECD 2012
  - C9 Aromatic Hydrocarbon Solvents category members are not expected to bioaccumulate based on BCF values from 23-342 for category members 1,2,4-trimethylbenzene and 1,3,5-

trimethylbenzene.

- U.S. EPA 2012
    - BCFBAF predicts a BCF of 177 based on a measured log K_{ow} of 3.30 (Appendix D).

Physical Hazards (Physical)

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: Japan METI/MOE* - GHS Classifications (GHS-Japan) Flammable liquids - Category 1
    - *Screening:* Québec CSST - WHMIS Classifications (WHMIS) Class B3 - Combustible liquids

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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 Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6)

TOXSERVICES TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

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	**Aromatic 100**	**6474-2-95-6**	**H**	**H**	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	**H**	**M**	**vL**	**L**	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
Aromatic 100	1

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

Table 6

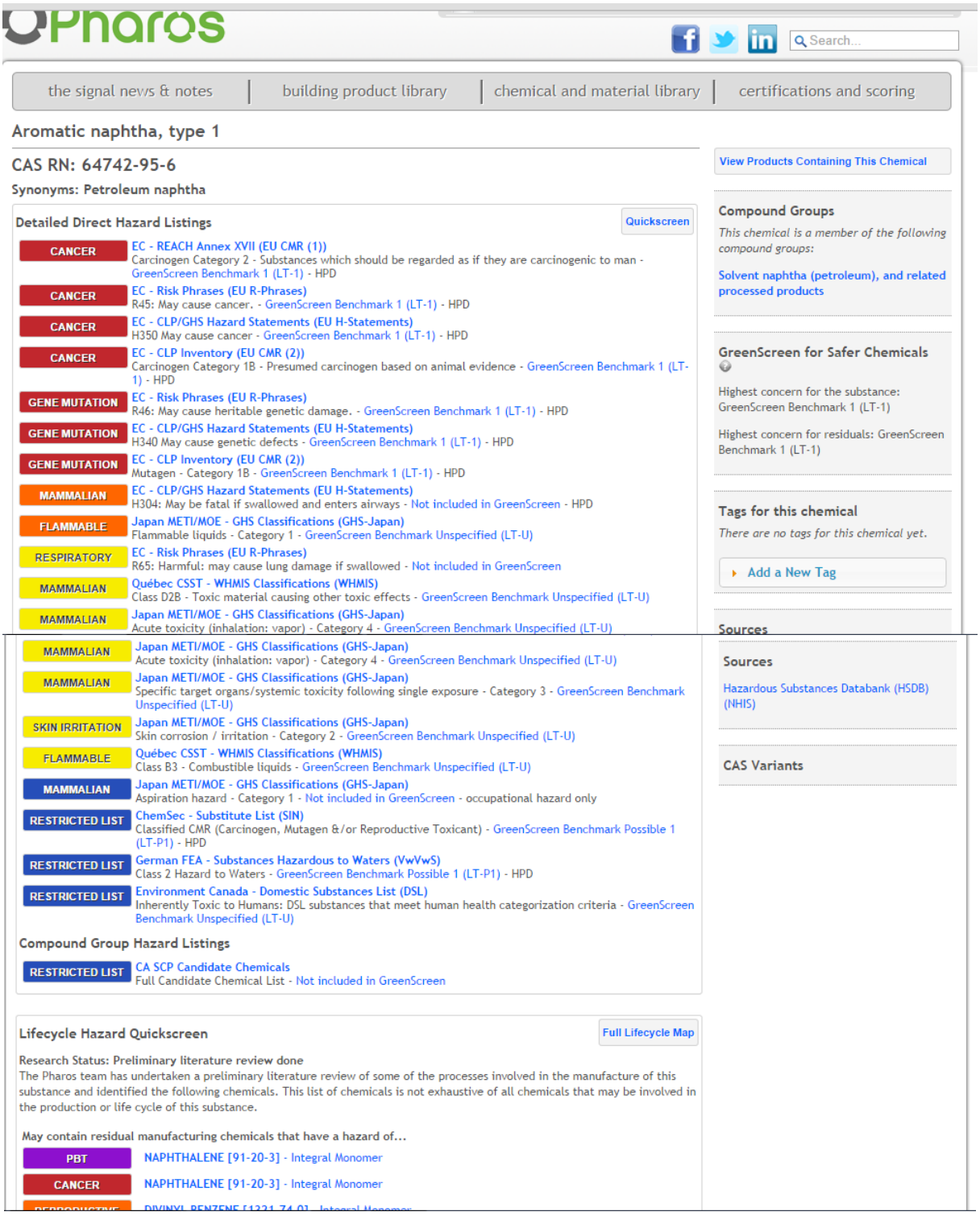
Chemical Name	Final GreenScreen® Benchmark Score
Aromatic 100	1

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 Aromatic 100 (Aromatic naphtha, type 1) (CAS# 64742-95-6)



Pharos

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Aromatic naphtha, type 1

CAS RN: 64742-95-6

Synonyms: Petroleum naphtha

Detailed Direct Hazard Listings — Quickscreen

CANCER	EC - REACH Annex XVII (EU CMR (1)) — Carcinogen Category 2 - Substances which should be regarded as if they are carcinogenic to man - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - Risk Phrases (EU R-Phrases) — R45: May cause cancer. - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - CLP/GHS Hazard Statements (EU H-Statements) — H350 May cause cancer - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - CLP Inventory (EU CMR (2)) — Carcinogen Category 1B - Presumed carcinogen based on animal evidence - GreenScreen Benchmark 1 (LT-1) - HPD
GENE MUTATION	EC - Risk Phrases (EU R-Phrases) — R46: May cause heritable genetic damage. - GreenScreen Benchmark 1 (LT-1) - HPD
GENE MUTATION	EC - CLP/GHS Hazard Statements (EU H-Statements) — H340 May cause genetic defects - GreenScreen Benchmark 1 (LT-1) - HPD
GENE MUTATION	EC - CLP Inventory (EU CMR (2)) — Mutagen - Category 1B - GreenScreen Benchmark 1 (LT-1) - HPD
MAMMALIAN	EC - CLP/GHS Hazard Statements (EU H-Statements) — H304: May be fatal if swallowed and enters airways - Not included in GreenScreen - HPD
FLAMMABLE	Japan METI/MOE - GHS Classifications (GHS-Japan) — Flammable liquids - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
RESPIRATORY	EC - Risk Phrases (EU R-Phrases) — R65: Harmful: may cause lung damage if swallowed - Not included in GreenScreen
MAMMALIAN	Québec CSST - WHMIS Classifications (WHMIS) — Class D2B - Toxic material causing other toxic effects - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) — Acute toxicity (inhalation: vapor) - Category 4 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) — Acute toxicity (inhalation: vapor) - Category 4 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) — Specific target organs/systemic toxicity following single exposure - Category 3 - GreenScreen Benchmark Unspecified (LT-U)
SKIN IRRITATION	Japan METI/MOE - GHS Classifications (GHS-Japan) — Skin corrosion / irritation - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	Québec CSST - WHMIS Classifications (WHMIS) — Class B3 - Combustible liquids - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) — Aspiration hazard - Category 1 - Not included in GreenScreen - occupational hazard only
RESTRICTED LIST	ChemSec - Substitute List (SIN) — Classified CMR (Carcinogen, Mutagen &/or Reproductive Toxicant) - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
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 to Humans: DSL substances that meet human health categorization criteria - GreenScreen Benchmark Unspecified (LT-U)

Compound Group Hazard Listings

RESTRICTED LIST	CA SCP Candidate Chemicals — Full Candidate Chemical List - Not included in GreenScreen

Lifecycle Hazard Quickscreen — Full Lifecycle Map

Research Status: Preliminary literature review done

The Pharos team has undertaken a preliminary literature review of some of the processes involved in the manufacture of this substance and identified the following chemicals. This list of chemicals is not exhaustive of all chemicals that may be involved in the production or life cycle of this substance.

May contain residual manufacturing chemicals that have a hazard of...

PBT	NAPHTHALENE [91-20-3] - Integral Monomer
CANCER	NAPHTHALENE [91-20-3] - Integral Monomer

View Products Containing This Chemical

Compound Groups

This chemical is a member of the following compound groups:

Solvent naphtha (petroleum), and related processed products

GreenScreen for Safer Chemicals

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

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

Tags for this chemical

There are no tags for this chemical yet.

Add a New Tag

Sources

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants

APPENDIX D: EPISuite Modeling Results for Aromatic 100 (Aliphatic naphtha, type 1) (CAS #64742-95-6)

CAS Number: 64742-95-6
SMILES: c12ccccc1cccc2
CHEM: Solvent naphtha (petroleum), light 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 (expkow 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/µg)):
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):
K_{oc}: 1544 L/kg (MCI method)
Log K_{oc}: 3.189 (MCI method)
K_{oc}: 730.6 L/kg (K_{ow} method)
Log K_{oc}: 2.864 (K_{ow} method)
Experimental Log K_{oc}: 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 (expk_{ow} 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

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