Naphthalene (CAS# 91-20-3) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

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GreenScreen® Executive Summary for Naphthalene (CAS# 91-20-3)

Naphthalene is a chemical that is used to manufacture chemicals that are used as softeners in polyvinyl chloride (PVC) plastics. Its major consumer uses are in insect and animal repellents, toilet deodorant blocks, synthetic tanning, preservative, textile chemicals, emulsion breakers, scintillation counters, and antiseptic (HSDB 2014).

Naphthalene 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)) This corresponds to GreenScreen® benchmark classification 1e in CPA 2011. Additional authoritative A listings were sufficient to assign hazard scores for acute toxicity (AT), acute aquatic toxicity (AA), chronic aquatic toxicity (CA), and flammability (F).

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 naphthalene did not identify any additional Benchmark 1 score 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 Naphthalene

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	NA	NA	NA	NA	**M**	NA	NA	NA	NA	NA	NA	NA	NA	**vH**	**M**	*H*	**M**	NA	M

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 Naphthalene (CAS# 91-20-3)

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

Chemical Name: Naphthalene

CAS Number: 91-20-3

GreenScreen® Assessment Prepared By:
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Organization: ToxServices LLC
Date: October 14, 2014
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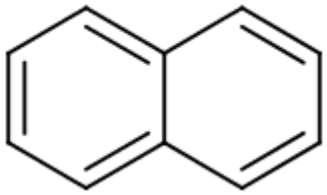
Name: Bingxuan Wang, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: December 1, 2014;

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

Chemical Structure(s):



Also called: EINECS 202-049-5, Albocarbon, camphor tar, Caswell No. 587, Mighty 150, Mighty RD1, Moth balls/Moth flakes, Naftalene, naphthalene, naphtalinum, naphthalin, naphthaline, naphthalinum, naphthene, white tar (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
No surrogates were used as Naphthalene is an LT-1 chemical.

Identify Applications/Functional Uses:
1. Insect and animal repellant
2. Deodorant
3. Fumigant
4. Manufacture of chemicals that are used as softeners in polyvinyl chloride (PVC) plastics

[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

5. Synthetic tanning
6. Preservative
7. Textile chemicals
8. Emulsion breakers
9. Scintillation counters
10. Antiseptic

GreenScreen® Summary Rating for Naphthalene[4]: Naphthalene 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)) This corresponds to GreenScreen® benchmark classification 1e in CPA 2011, 2012a. Additional authoritative A listings were sufficient to assign hazard scores for acute toxicity (AT), acute aquatic toxicity (AA), chronic aquatic toxicity (CA), and flammability (F). 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 naphthalene did not identify any additional Benchmark 1 score combinations.

Figure 1: GreenScreen® Hazard Ratings for Naphthalene

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	NA	NA	NA	NA	M	NA	NA	NA	NA	NA	NA	NA	NA	vH	M	*H*	M	NA	M

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 Naphthalene is an LT-1 chemical and its score will not be impacted by those of transformation products.

[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.

Introduction

Naphthalene is a chemical that is used to manufacture chemicals that are used as softeners in polyvinyl chloride (PVC) plastics. Its major consumer uses are in insect and animal repellents, toilet deodorant blocks, synthetic tanning, preservative, textile chemicals, emulsion breakers, scintillation counters, and antiseptic (HSDB 2014).

ToxServices assessed Naphthalene 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 Naphthalene can be found in Appendix C and a summary of the results can be found below:

- Carcinogenicity
  - US NIH – Report on Carcinogens – Reasonably Anticipated to be a Human Carcinogen
  - Cal/EPA – Chemicals Known to Cause Cancer & Reproductive Toxicity (Prop 65) - Cancer
  - German MAK – Carcinogen Group 2 – considered to be carcinogenic to man
  - EU Risk Phrase R40 – limited evidence of carcinogenic effect
  - US EPA/IRIS – (1986) Group C – possible carcinogen
  - IARC – Group 2b – possibly carcinogenic to humans
  - GHS Hazard Statement H351 – suspected of causing cancer
  - EC - CLP Inventory (EU CMR (2)) Carcinogen Category 2 - Suspected human carcinogen
  - GHS-New Zealand 6.7B (Category 2) – suspected human carcinogen
  - GHS-Japan – Category 2 – Carcinogenicity 2
  - US EPA – PPT chemical action plans – Possible carcinogen – TSCA criteria met
  - US EPA/IRIS – (1996) carcinogenic potential cannot be determined
- Endocrine
  - ChemSec – Substitute List (SIN) - equivalent concern, including endocrine disruption - Sin List 1.0
- Gene mutation –
  - German MAK – 3b - Germ cell mutagen
- Mammalian
  - GHS-Japan – Category 1 – Specific target organs/systemic toxicity following single exposure
  - GHS-New Zealand - 6.9A (oral) (Category 1) - Specific Target Organ Systemic Toxicity (Single Exposure)
  - GHS-New Zealand - 6.9A (inhalation) (Category 1) - Specific Target Organ Systemic Toxicity (Single Exposure)
  - EU Risk Phrase R22 – Harmful if swallowed
  - GHS Hazard Statement H302 – Harmful if swallowed

    - Québec CSST - WHMIS Classifications (WHMIS) Class D2A - Very toxic material causing other toxic effect
    - GHS-New Zealand 6.1D (Category 4) – acutely toxic (dermal)
    - GHS-New Zealand 6.1D (Category 4) –acutely toxic (oral)
    - GHS-Japan – Category 4 – Acutely toxic
    - GHS-Japan – Category 1 – specific target organs/systemic toxicity following repeated exposure
- Skin Sensitization
    - GHS-Japan – Category 1 – skin sensitizer
- Skin irritation
    - GHS-New Zealand 6.3B (Category 2A) – mildly irritating to the skin
    - GHS-Japan – Category 3 – skin corrosion/irritation
- Eye irritation
    - GHS-New Zealand 6.4A (Category 3) – irritating to the eye
    - GHS-Japan – Category 3 – serious eye damage/eye irritation
- Acute Aquatic
    - GHS Hazard Statement H400 – Aquatic Acute 1 – very toxic to aquatic life
    - EU Risk Phrase R50 – very toxic to aquatic organisms
    - GHS-New Zealand 9.1A (Category 1) – very ecotoxic in aquatic environment (algal)
    - GHS-Japan – Category 1 – Hazardous to the aquatic environment (acute)
- Chronic Aquatic
    - GHS Hazard Statement H410 – Aquatic Chronic 1 – very toxic to aquatic life with long lasting effects
    - GHS-Japan – Category 1 – hazardous to the aquatic environment (chronic)
    - EU Risk Phrase R53 – may cause long-term adverse effects in the aquatic environment
    - GHS-New Zealand 9.1B (Category 2) - very ecotoxic in the aquatic environment (crustacean)
    - GHS-New Zealand 9.1B (Category 2) - very ecotoxic in the aquatic environment (fish)
- PBT
    - US EPA – Priority PBT (NWMP Priority)[6]
    - US EPA – low bioaccumulation potential
    - US EPA – low environmental potential
- Flammable
    - US DOT IMO – Group III Class 4.1 - flammable solid
    - Québec CSST - WHMIS Classifications (WHMIS) Class B4- Flammable solids
    - GHS- New Zealand 4.1.1B - (Category 2) – Flammable solids
    - GHS-Japan – Category 2 – flammable solid
- Restricted List
    - German FEA – (VwVwS) Class 3 severe hazard to waters
    - US EPA – Hazardous Air Pollutant
    - US OSHA - Carcinogen
    - Environment Canada – CEPA Toxic
    - Environment Canada – DSL inherently toxic to humans
    - Environment Canada – DSL inherently toxic to environment

[6] Classification by U.S. EPA as a Priority PBT (NWMP Priority) corresponds to a score of LT-1. However, as this listing does not correspond directly to hazard classifications for specific endpoints and results from a GreenScreen® assessment always take priority over results from the List Translator, this classification alone was not used to assign the Benchmark score.

PhysicoChemical Properties of Naphthalene

Naphthalene is polyaromatic hydrocarbon solid. It has a vapor pressure of 0.085 mm Hg indicating that it will likely exist in the solid phases; however, it has a low melting point and sublimates easily. 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; which correlates to the high BCF values of 36.5-714.

Table 1: Physical and Chemical Properties of Naphthalene (CAS# 91-20-3)

Property	Value	Reference
Molecular formula	C10-H8	ChemIDplus 2014
SMILES Notation	c12c(cccc1)cccc2	ChemIDplus 2014
Molecular weight	128.173	ChemIDplus 2014
Physical state	Solid	HSBD 2014
Appearance	White crystalline flakes	HSDB 2014
Melting point	80.2°C	HSDB 2014
Vapor pressure	0.085 mm Hg at 25°C	HSDB 2014
Water solubility	31 mg/L at 25ºC	HSDB 2014
Dissociation constant	Not identified	
Density/specific gravity	1.162 at 20ºC	HSDB 2014
Partition coefficient	Log K_{ow} = 3.30	HSDB 2014

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): H

Naphthalene 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 NIH RoC, Cal/EPA Prop 65, and German MAK (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* US NIH – Report on Carcinogens – reasonably anticipated to be a Human Carcinogen
    - *Authoritative:* Cal/EPA – Chemicals Known to Cause Cancer & Reproductive Toxicity (Prop 65) - Cancer
    - *Authoritative:* German MAK – Carcinogen Group 2 – Considered to be carcinogenic to man
    - *Authoritative:* EU Risk Phrase R40 – limited evidence of carcinogenic effect
    - *Authoritative:* US EPA/IRIS (1986) – Group C – Possible carcinogen
    - *Authoritative:* IARC – Group 2b – possibly carcinogenic to humans
    - *Authoritative:* GHS Hazard Statement H351 – suspected of causing cancer
    - *Authoritative:* EC - CLP Inventory (EU CMR (2)) Carcinogen Category 2 - Suspected human carcinogen
    - *Authoritative:* US EPA/IRIS – (1996) carcinogenic potential cannot be determined
    - *Screening:* GHS-New Zealand 6.7B (Category 2) – Suspected human carcinogen
    - *Screening:* GHS-Japan – Category 2 – Carcinogenicity 2

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

- *Authoritative:* German MAK – 3b - Germ cell 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:* ChemSec – Substitute List (SIN) - equivalent concern, including endocrine disruption - Sin List 1.0
- High Throughput Screening (HTS) Data –
  - HTS data were identified for naphthalene using PubChem (http://pubchem.ncbi.nlm.nih.gov/).
  - The data included the following results:
    - Naphthalene was active in 0/11 androgen receptor agonist assays and 0/20 androgen receptor antagonist assays.
    - Naphthalene was active in 0/11 estrogen receptor-alpha agonist assays and 0/20 estrogen receptor-alpha antagonist assays.
    - Naphthalene was active in 0/5 thyroid receptor agonist assays and 0/11 thyroid receptor antagonist assays.
    - Naphthalene was active in 0/3 thyroid stimulating hormone receptor agonist assays and 0/1 thyroid stimulating hormone receptor antagonist assay.
- These data are insufficient to assign a score for endocrine activity.

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): M

Naphthalene was assigned a score of Moderate for acute toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Moderate hazard for acute toxicity when the chemical has GHS Hazard Statement H302 (CPA 2012a).

- *Authoritative:* EU Risk Phrase R22 – Harmful if swallowed
- *Authoritative:* GHS Hazard Statement H302 – Harmful if swallowed
- Québec CSST - WHMIS Classifications (WHMIS) Class D2A - Very toxic material causing other toxic effect

- *Screening:* GHS-New Zealand 6.1D (Category 4) –acutely toxic (oral)
- *Screening:* GHS-New Zealand 6.1D (Category 4) – acutely toxic (dermal)
- *Screening:* GHS-Japan – Category 4 – Acutely toxic

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:* GHS-Japan – Category 1 – Specific target organs/systemic toxicity following repeated exposure

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* GHS-New Zealand - 6.9A (oral) (Category 1) - Specific Target Organ Systemic Toxicity (Single Exposure)
  - *Screening:* GHS-New Zealand - 6.9A (inhalation) (Category 1) - Specific Target Organ Systemic Toxicity (Single Exposure)
  - *Screening:* GHS-Japan – Category 1 – Specific target organs/systemic toxicity following single exposure

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:* GHS-Japan – Category 1 – skin sensitizer

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:* GHS-New Zealand 6.3B (Category 2A) – mildly irritating to the skin
  - *Screening:* GHS-Japan – Category 3 – skin corrosion/irritation

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:* GHS-New Zealand 6.4A (Category 3) – serious eye damage
    - *Screening:* GHS-Japan – Category 3 – serious eye damage/eye irritation

Ecotoxicity (Ecotox)

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

Naphthalene was assigned a score of Very High for acute aquatic toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Very High for acute aquatic toxicity when the chemical has EU Risk Phrase R50 and GHS Hazard Statement H400 (CPA 2012a).

- *Authoritative:* GHS Hazard Statement H400 – Aquatic Acute 1 – very toxic to aquatic life
- *Authoritative:* EU Risk Phrase R50 – very toxic to aquatic organisms
- *Screening:* GHS-New Zealand 9.1A (Category 1) – very ecotoxic in aquatic environment (algal)
- *Screening:* GHS-Japan – Category 1 – Hazardous to the aquatic environment (acute)

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

Naphthalene was assigned a score of Moderate for chronic aquatic toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Moderate for chronic aquatic toxicity when the chemical has EU Risk Phrase R53 (CPA 2012a).

- *Authoritative:* GHS Hazard Statement H410 – Aquatic Chronic 1 – very toxic to aquatic life with long lasting effects
- *Authoritative:* EU Risk Phrase R53 – may cause long-term adverse effects in the aquatic environment
- *Screening:* GHS-Japan – Category 1 – hazardous to the aquatic environment (chronic)
- *Screening:* GHS-New Zealand 9.1B (Category 2) - very ecotoxic in the aquatic environment (crustacean)
- *Screening:* GHS-New Zealand 9.1B (Category 2) - very ecotoxic in the aquatic environment (fish)

Environmental Fate (Fate)

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

Naphthalene was assigned a score of High for persistence based on a predicted half-life of 75 days in soil. GreenScreen® criteria classify chemicals as a High hazard for persistence when there is a half-life of 60-180 days in the soil compartment (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* US EPA – Priority PBT
    - *Screening:* US EPA – low bioaccumulation potential
    - *Screening:* US EPA – low environmental potential
- ECHA 2014
    - In a non-GLP-compliant inherent biodegradation study similar to OECD Guideline 302C (Inherent Biodegradability: Modified MITI Test (II)) using activated sludge inoculum, naphthahlene (30 ppm starting concentration, purity not specified) there was no biodegradation observed. Authors concluded that the substance is not biodegradable.

- EC 2003
    - The fate of naphthalene in a wastewater treatment plant is 27.4% to air, 34.8% to water, 11.2% to sludge, and 26.6% degraded.
    - 96.8% of influent naphthalene was removed from a municipal treatment plant.
    - A batch reactor filled with acclimated sludge, mineral salts, and naphthalene was used to follow the degradation of naphthalene under aerobic conditions. Depending on the initial concentration (5-25 mg/L), up to 99% naphthalene was degraded in 2.8-8 hours.
    - Naphthalene was not readily biodegradable, with 2% degradation occurring in 28 days in OECD 301C (Ready Biodegradability: Modified MITI test (I) and OECD 302C (Inherent Biodegradability: Modified MITI test (II)).
- U.S. EPA 2012
    - The BIOWIN modeling Ready Biodegradable Predictor indicates that naphthalene 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 37.5 days, and 0.998% will partition to sediment with a half-life of 337.5 days (Appendix D).
- A weight of evidence approach was taken due to the varying reported levels of persistence. It is neither readily nor inherently biodegradable in OECD guideline studies, but biodegrades in treatment facilities. Modeling predicts that naphthalene is not readily biodegradable, with a half-life of 75 days in its predicted major compartment of soil; this conflicts with the fate of naphthalene in a treatment plant, where the major compartment is water. Based on the variation in data, the conservative half-life value of 75 days in soil is being used to assign the hazard score.

Bioaccumulation (B) Score (vH, H, M, L, or vL): M
Naphthalene was assigned a score of Moderate for bioaccumulation based on the highest BCF of 714 in fish. GreenScreen® criteria classify chemicals as a Moderate hazard for bioaccumulation when BCF values are between 500 and 1,000 (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* US EPA – Priority PBT
    - *Screening:* US EPA – low bioaccumulation potential
    - *Screening:* US EPA – low environmental potential
- ECHA 2014
    - A BCF of 23-168 was established in an eight week flow-through study conducted according to OECD Guideline 305 (Bioconcentration: Flow-through Fish Test) in *Cyprinus carpio*.
    - BCF values of 30 and 95 were established in *Onchorynchus kisutch* (coho salmon) and *Platichthys stellatus* (starry flounder) in a six week flow-through study conducted according to OECD Guideline 305 (Bioconcentration: Flow-through Fish Test).
- HSDB 2014
    - The experimental BCF values in sheepshead minnows (*Cyprinodon variegatus*) exposed to 1.34 and 12.5 ug/L naphthalene for 36 days were 692 and 714.
    - The experimental BCF values in amphipods (*Diporeia spp)* exposed to 453.2 to 2201.1 ug/L naphthalene for 28 days were 490 to 736

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): M

Naphthalene was assigned a score of Moderate for flammability based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Moderate for flammability when the chemical is classified as a flammable solid WHMIS Class B4 (CPA 2012a).

- *Authoritative:* US DOT IMO – Group III Class 4.1 - flammable solid
- *Authoritative:* Québec CSST - WHMIS Classifications (WHMIS) Class B4- Flammable solids
- *Screening:* GHS- New Zealand 4.1.1B - (Category 2) – Flammable solids
- *Screening:* GHS-Japan – Category 2 – flammable solid

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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 Naphthalene (CAS# 91-20-3)

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	**Naphthalene**	**91-20-3**	H	DG	DG	DG	DG	M	DG	DG	DG	DG	DG	DG	DG	DG	vH	M	*H*	**M**	DG	M

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
Naphthalene	1

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

Table 6

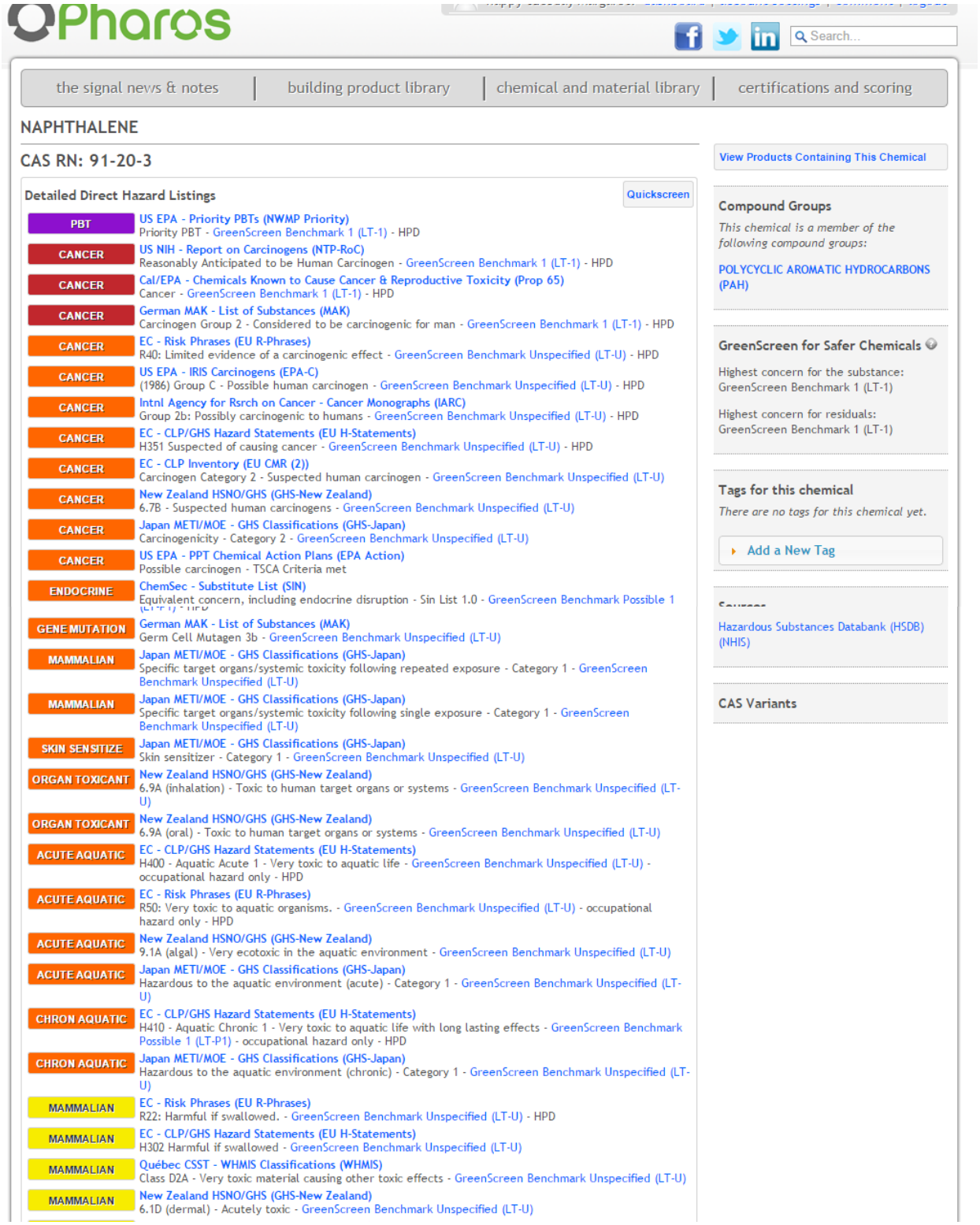
Chemical Name	Final GreenScreen® Benchmark Score
Naphthalene	1

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 Naphthalene (CAS# 91-20-3)



Pharos

Search...

the signal news & notes | building product library | chemical and material library | certifications and scoring

NAPHTHALENE

CAS RN: 91-20-3

View Products Containing This Chemical

Detailed Direct Hazard Listings — Quickscreen

PBT	US EPA - Priority PBTs (NWMP Priority) Priority PBT - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	US NIH - Report on Carcinogens (NTP-RoC) Reasonably Anticipated to be Human Carcinogen - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	Cal/EPA - Chemicals Known to Cause Cancer & Reproductive Toxicity (Prop 65) Cancer - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	German MAK - List of Substances (MAK) Carcinogen Group 2 - Considered to be carcinogenic for man - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - Risk Phrases (EU R-Phrases) R40: Limited evidence of a carcinogenic effect - GreenScreen Benchmark Unspecified (LT-U) - HPD
CANCER	US EPA - IRIS Carcinogens (EPA-C) (1986) Group C - Possible human carcinogen - GreenScreen Benchmark Unspecified (LT-U) - HPD
CANCER	Intnl Agency for Rsrch on Cancer - Cancer Monographs (IARC) Group 2b: Possibly carcinogenic to humans - GreenScreen Benchmark Unspecified (LT-U) - HPD
CANCER	EC - CLP/GHS Hazard Statements (EU H-Statements) H351 Suspected of causing cancer - GreenScreen Benchmark Unspecified (LT-U) - HPD
CANCER	EC - CLP Inventory (EU CMR (2)) Carcinogen Category 2 - Suspected human carcinogen - GreenScreen Benchmark Unspecified (LT-U)
CANCER	New Zealand HSNO/GHS (GHS-New Zealand) 6.7B - Suspected human carcinogens - GreenScreen Benchmark Unspecified (LT-U)
CANCER	Japan METI/MOE - GHS Classifications (GHS-Japan) Carcinogenicity - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
CANCER	US EPA - PPT Chemical Action Plans (EPA Action) Possible carcinogen - TSCA Criteria met
ENDOCRINE	ChemSec - Substitute List (SIN) Equivalent concern, including endocrine disruption - Sin List 1.0 - GreenScreen Benchmark Possible 1
GENE MUTATION	German MAK - List of Substances (MAK) Germ Cell Mutagen 3b - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following repeated exposure - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
SKIN SENSITIZE	Japan METI/MOE - GHS Classifications (GHS-Japan) Skin sensitizer - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
ORGAN TOXICANT	New Zealand HSNO/GHS (GHS-New Zealand) 6.9A (inhalation) - Toxic to human target organs or systems - GreenScreen Benchmark Unspecified (LT-U)
ORGAN TOXICANT	New Zealand HSNO/GHS (GHS-New Zealand) 6.9A (oral) - Toxic to human target organs or systems - GreenScreen Benchmark Unspecified (LT-U)
ACUTE AQUATIC	EC - CLP/GHS Hazard Statements (EU H-Statements) H400 - Aquatic Acute 1 - Very toxic to aquatic life - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only - HPD
ACUTE AQUATIC	EC - Risk Phrases (EU R-Phrases) R50: Very toxic to aquatic organisms. - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only - HPD
ACUTE AQUATIC	New Zealand HSNO/GHS (GHS-New Zealand) 9.1A (algal) - Very ecotoxic in the aquatic environment - GreenScreen Benchmark Unspecified (LT-U)
ACUTE AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan) Hazardous to the aquatic environment (acute) - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	EC - CLP/GHS Hazard Statements (EU H-Statements) H410 - Aquatic Chronic 1 - Very toxic to aquatic life with long lasting effects - GreenScreen Benchmark Possible 1 (LT-P1) - occupational hazard only - HPD
CHRON AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan) Hazardous to the aquatic environment (chronic) - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	EC - Risk Phrases (EU R-Phrases) R22: Harmful if swallowed. - GreenScreen Benchmark Unspecified (LT-U) - HPD
MAMMALIAN	EC - CLP/GHS Hazard Statements (EU H-Statements) H302 Harmful if swallowed - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Québec CSST - WHMIS Classifications (WHMIS) Class D2A - Very toxic material causing other toxic effects - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	New Zealand HSNO/GHS (GHS-New Zealand) 6.1D (dermal) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)

Compound Groups

This chemical is a member of the following compound groups:

POLYCYCLIC AROMATIC HYDROCARBONS (PAH)

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

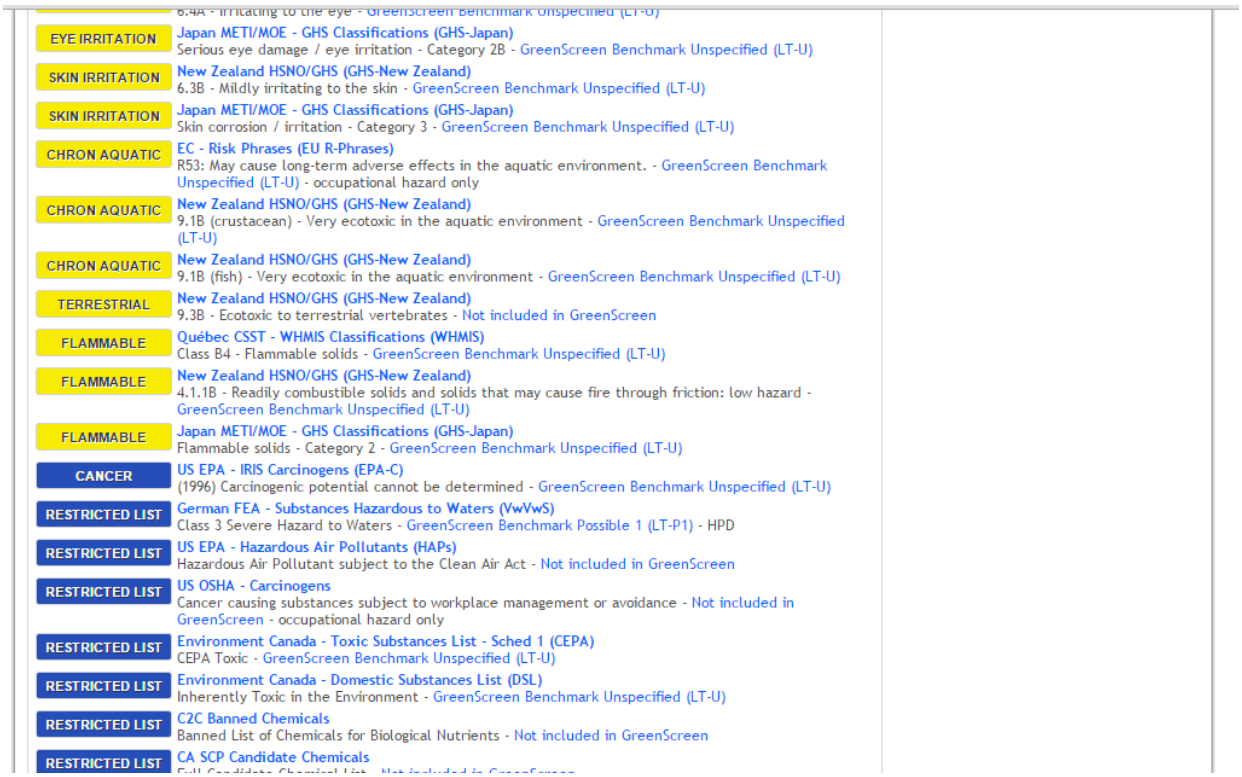
There are no tags for this chemical yet.

Add a New Tag

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants



	6.4A - Irritating to the eye - GreenScreen Benchmark Unspecified (LT-U)
EYE IRRITATION	Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2B - GreenScreen Benchmark Unspecified (LT-U)
SKIN IRRITATION	New Zealand HSNO/GHS (GHS-New Zealand) 6.3B - Mildly irritating to the skin - GreenScreen Benchmark Unspecified (LT-U)
SKIN IRRITATION	Japan METI/MOE - GHS Classifications (GHS-Japan) Skin corrosion / irritation - Category 3 - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	EC - Risk Phrases (EU R-Phrases) R53: May cause long-term adverse effects in the aquatic environment. - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only
CHRON AQUATIC	New Zealand HSNO/GHS (GHS-New Zealand) 9.1B (crustacean) - Very ecotoxic in the aquatic environment - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	New Zealand HSNO/GHS (GHS-New Zealand) 9.1B (fish) - Very ecotoxic in the aquatic environment - GreenScreen Benchmark Unspecified (LT-U)
TERRESTRIAL	New Zealand HSNO/GHS (GHS-New Zealand) 9.3B - Ecotoxic to terrestrial vertebrates - Not included in GreenScreen
FLAMMABLE	Québec CSST - WHMIS Classifications (WHMIS) Class B4 - Flammable solids - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	New Zealand HSNO/GHS (GHS-New Zealand) 4.1.1B - Readily combustible solids and solids that may cause fire through friction: low hazard - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	Japan METI/MOE - GHS Classifications (GHS-Japan) Flammable solids - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
CANCER	US EPA - IRIS Carcinogens (EPA-C) (1996) Carcinogenic potential cannot be determined - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	German FEA - Substances Hazardous to Waters (VwVwS) Class 3 Severe Hazard to Waters - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
RESTRICTED LIST	US EPA - Hazardous Air Pollutants (HAPs) Hazardous Air Pollutant subject to the Clean Air Act - Not included in GreenScreen
RESTRICTED LIST	US OSHA - Carcinogens Cancer causing substances subject to workplace management or avoidance - Not included in GreenScreen - occupational hazard only
RESTRICTED LIST	Environment Canada - Toxic Substances List - Sched 1 (CEPA) CEPA Toxic - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	Environment Canada - Domestic Substances List (DSL) Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	C2C Banned Chemicals Banned List of Chemicals for Biological Nutrients - Not included in GreenScreen
RESTRICTED LIST	CA SCP Candidate Chemicals Full Candidate Chemical List - Not included in GreenScreen

APPENDIX D: EPISuite Modeling Results for Naphthalene (CAS #91-20-3)

CAS Number: 91-20-3
SMILES: c(c(ccc1)ccc2)(c1)c2
CHEM: Naphthalene
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/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: 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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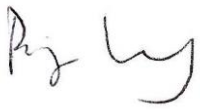

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