Stoddard solvent (CAS# 8052-41-3) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

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GreenScreen® Executive Summary for Stoddard Solvent (CAS# 8052-41-3)

Stoddard solvent is a chemical that functions as diluent in paints, coatings and waxes; as a dry-cleaning agent; as a vehicle for various lipophilic pesticides; and as a degreaser and cleaner in mechanical shops (HSDB 2014).

Stoddard solvent 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. Additional authoritative A listings were sufficient to assign a score of Moderate for systemic toxicity repeated dose (STr*), and a score of High for flammability (F). As Stoddard solvent is an LT-1 chemical assessment of additional endpoints was not performed.

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 Stoddard solvent results in the capture of an additional Benchmark 1 combination of 1d, due to Very High bioaccumulation (B).

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 Stoddard Solvent

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

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 Stoddard Solvent (CAS# 8052-41-3)

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

Chemical Name: Stoddard solvent

CAS Number: 8052-41-3

GreenScreen® Assessment Prepared By:
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Date: October 16, 2014
Assessor Type: Licensed GreenScreen® Profiler

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

Chemical Structure(s):
No structure identified for this complex mixture of hydrocarbons. It is a variable mixture of aliphatic hydrocarbon molecules with carbon numbers ranging from 9 to 14 and contains a large number of constituents including n-paraffins (n-alkanes), iso-paraffins (isoalkanes), cyclic-paraffins or naphthenic (cyclics), and aromatics. It includes C8 to C14 branched, linear, and cyclic paraffins and aromatics (6 to 18%), <50ppmV benzene (OECD 2012)

Also called: Caswell No. 802; EINECS 232-489-3; EPA Pesticide Chemical Code 063504; HSDB 7171; Naphtha, solvent; Petroleum distillates; UNII-37LNJ1I16R; White spirit (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Stoddard solvent is a member of OECD's C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category, which are all variable mixtures of aliphatic hydrocarbon molecules with carbon numbers ranging from 9 to 14 (OECD 2012). Due to similar composition, data for other category members and read-across chemicals from this category were used as surrogates.

Identify Applications/Functional Uses:
1. Solvent,

[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

2. Diluent in paints,
3. Coatings and waxes,
4. Dry-cleaning agent,
5. Lipophilic pesticides, and
6. Degreaser and cleaner in mechanical shops

GreenScreen® Summary Rating for Stoddard Solvent[4]:

Stoddard solvent 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, 2012a. Additional authoritative A listings were sufficient to assign a score of Moderate for systemic toxicity repeated dose (STr*), and a score of High for flammability (F). As Stoddard solvent is an LT-1 chemical assessment of additional endpoints was not performed. 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 Stoddard solvent results in the capture of an additional Benchmark 1 combination of 1d, due to Very High bioaccumulation (B).

Figure 1: GreenScreen® Hazard Ratings for Stoddard Solvent

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

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]

[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.

Transformation products were not assessed, as Stoddard solvent is an LT-1 chemical and its score will not be impacted by those of transformation products.

Introduction

Stoddard solvent is a mixture of straight & branched chain paraffins, naphthenes Assoc (cycloparaffins) & alkyl aromatic hydrocarbons. A colorless, refined petroleum distillate that is free from rancid or objectionable odors and that boils in the range of approximately 149°C to 204.5°C (300°F to 400°F) (ChemIDplus 2014). Stoddard solvent functional uses are as follows: diluent in paints; coatings and waxes; as a dry-cleaning agent; as a vehicle for various lipophilic pesticides; and as a degreaser and cleaner in mechanical shops (HSDB 2014).

ToxServices assessed Stoddard solvent 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 Stoddard solvent 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
  - GHS Hazard Statement H372 – Causes damage to organs through prolonged or repeated exposure
  - EU Risk Phrase R65 – Harmful: may cause lung damage if swallowed
  - Canada WHMIS – Class D2B - Toxic material causing other toxic effects
  - GHS-Japan – Category 2 - Systemic toxicity following repeated exposure
  - GHS-Japan – Category 3 - Systemic toxicity following single exposure
  - GHS-New Zealand - 6.1E (oral) (Category 5)– Acutely toxic
  - GHS-Japan – Category 1 – Aspiration hazard
- Neurotoxicity
  - Patty's Toxicity – Boyes Neurotoxicants - Neurotoxic
- Skin irritation
  - GHS-New Zealand - 6.3B (Category 3) – Mildly irritating to the skin
  - GHS-Japan – Category 2 – Skin corrosion/irritation

- Flammable
  - US DOT – Class 3 Group II - flammable liquid
  - Canada WHMIS – Class B3 – combustible liquid
  - GHS-New Zealand – 3.1C (Category 3)– flammable liquid: medium hazard
- Aquatic
  - GHS-Japan – Category 1 – hazardous to the aquatic environment (acute)
  - GHS-Japan – Category 1 – hazardous to the aquatic environment (chronic)
  - GHS-New Zealand – 9.1B (Category 2) – Very ecotoxic in the aquatic environment (chronic)
- PBT
  - Canada – DSL – substances that are bioaccumulative
- Restricted List
  - German FEA – (VwVwS) Class 2 Hazard to water
  - Environment Canada – DSL inherently toxic to humans
  - Environment Canada – DSL inherently toxic to environment
  - CA SCP Candidate Chemicals – Initial and Full Candidate Chemical List

PhysicoChemical Properties of Stoddard Solvent

Stoddard solvent is a liquid petroleum mixture under standard temperature and pressure. It has a vapor pressure of 1.5 mm Hg 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 Stoddard Solvent (CAS# 8052-41-3)

Property	Value	Reference
Molecular formula	Mixture - variable	
SMILES Notation	Mixture - variable	
Molecular weight	140	HSDB 2014
Physical state	Liquid	HSDB 2014
Appearance	Colorless kerosene like odor	HSDB 2014
Melting point	-60°C	HSDB 2014
Vapor pressure	0.2 kPa (1.5 mm Hg) 25°C	HSDB 2014
Water solubility	0.01%	HSDB 2014
Dissociation constant	Not identified	
Density/specific gravity	0.75-0.85	HSDB 2014
Partition coefficient	log K_{ow} = 3.16-7.06	HSDB 2014
Bioavailability	Not identified	

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

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

Stoddard solvent 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
Stoddard solvent 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 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:* GHS-New Zealand - 6.1E (oral) (Category 5) – 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 3 - Specific target organs/systemic toxicity following single exposure

***Group II* Score (repeated dose)* (H, M, or L): M**
Stoddard solvent was assigned a score of Medium for systemic repeat dose toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Medium hazard for carcinogenicity when the chemical is associated with H372 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* GHS Hazard Statement H372 - Causes damage to organs through prolonged or repeated exposure
  - *Screening:* WHIMS - class D2B - Toxic material causing other toxic effects
  - *Screening:* GHS-Japan – Category 2 - Systemic toxicity following repeated 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:* Patty's Toxicology - Boyes Neurotoxicants: Neurotoxic
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Patty's Toxicology - Boyes Neurotoxicants: Neurotoxic
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

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

- Authoritative and Screening Lists
  - *Authoritative:* 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:* GHS-New Zealand - 6.3B – (Category 3) Mildly irritating to the skin
  - *Screening:* GHS-Japan – Category 2 – 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:* Not present on any screening lists

Ecotoxicity (Ecotox)

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

Stoddard solvent was assigned a score of High for acute aquatic toxicity based on LL/EL_{50} values of 3.5 mg/L in invertebrates and 2.5 mg/L in algae for Stoddard solvent, and LL_{50} values of 41.4 mg/L and 25 mg/L in fish for category members. GreenScreen® criteria classify chemicals as a High hazard for acute aquatic toxicity when acute aquatic toxicity values are between 1 and 10 mg/L.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* GHS-Japan – Category 1 – hazardous to the aquatic environment (acute)
  - *Screening:* Environment Canada – DSL inherently toxic to environment

Stoddard solvent (CAS# 8052-41-3)

- OECD 2012
  - 48-hour LL_{50} (*Chaetogammarus marinus*, sand shrimp) = 3.5 mg/L
  - 72-hour EL_{50} (*Pseudokirchneriella subcapitata*, green algae) = 2.5 mg/L (biomass), 5.5 mg/L (growth)
- NITE 1996
  - Stoddard solvent was classified as GHS Category 1 in Japan based on EC_{50} values of 0.42-2.3 mg/L in *Daphnia magna*.
- OECD 2014
  - Classification as inherently toxic to aquatic organisms is based on modeled LC/EC_{50} values. The pivotal value used for the classification is 0.61 mg/L.

C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category

- OECD 2012
  - 96-hour LL_{50} (freshwater fish) = 41.4 mg/L (CAS# 64742-82-1)
  - 48-hour EL_{50} (*Daphnia magna*, water flea) = 3-10 mg/L (CAS# 64742-82-1)
  - 72-hour EL_{50} (*Pseudokirchneriella subcapitata*, green algae) = 1-3 mg/L (biomass), 1-3 mg/L (growth) (CAS# 64742-82-1)
  - 96-hour LL_{50} (freshwater fish) = 25 mg/L (CAS# 64742-81-0)
  - 48-hour EL_{50} (*Daphnia magna*, water flea) = 1.4 mg/L(CAS# 64742-81-0)
  - 72-hour EL_{50} (*Pseudokirchneriella subcapitata*, green algae) = 8.3 mg/L (biomass), 15 mg/L (growth) (CAS# 64742-81-0)
- Based on the weight of evidence a score of High was assigned. The most conservative LL/EL_{50} values for Stoddard solvent are 3.5 mg/L in invertebrates and 2.5 mg/L in algae. Category members have LL_{50} values of 41.4 and 25 mg/L in fish. These values correspond to a score of High. The EL_{50} values of 1-3 mg/L in algae for category members were not used to assign a score of Very High, because measured data were available for Stoddard solvent indicate that a High is appropriate. GHS classification in Japan was not weighed heavily in the assessment, because it is based on EC_{50} rather than EL_{50} values, which are more appropriate for complex substances with a wide range of water solubility (UN 2013). Classification on the DSL was disregarded as it is based on modeled data, and measured data are available for this compound.

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

Stoddard solvent was assigned a score of High for chronic aquatic toxicity based on a NOEL of 0.28 mg/L in daphnia. GreenScreen® criteria classify chemicals as a High hazard for chronic aquatic toxicity when chronic aquatic toxicity values are between 0.1 and 1 mg/L (CPA 2012a).

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

  - *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 (chronic)
  - *Screening:* Environment Canada – DSL inherently toxic to environment

Stoddard solvent (CAS# 8052-41-3)

- OECD 2012
  - 72-hour NOEL (*Pseudokirchneriella subcapitata*, green algae) = 0.76 mg/L (biomass), 0.16 mg/L (growth)
  - 21-day NOEL (*Daphnia magna*, water flea = 1.4 mg/L (immobilization/growth), 0.28 mg/L (reproduction)
  - 96-hour NOEL (*Pseudokirchneriella subcapitata*, green algae) = 0.76 mg/L (biomass, growth)
- NITE 1996
  - Stoddard solvent was classified as GHS Category 1 in Japan based on classification of acute Category 1, not rapidly degrading, and unknown bioaccumulation potential.
- Based on the weight of evidence a score of High was assigned. As explained above, the classification on the DSL is based on modeled data which was disregarded in favor of measured data. Available NOEC values correspond to a score of High.

Environmental Fate (Fate)

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

Stoddard solvent was assigned a score of Very Low for persistence based on positive results in a ready biodegradability assay for a compositionally similar category member, and modeling results predicting that it partitions primarily to water and is readily biodegradable. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence if the chemical partitions primarily to water and meets the 10-day window (CPA 2012a).

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

Stoddard solvent (CAS# 8052-41-3)

- U.S. EPA 2012
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that Stoddard solvent is expected to be readily biodegradable. Fugacity modeling predicts 69.1% will partition to water with a half-life of 9 days, 26.9% will partition to air with a half-life of 22.1 hours, and 2.27% will partition to sediment with a half-life of 78 days (Appendix D). ToxServices noted that the default structure associated with this CAS number is a straight chain carbohydrate containing 10 carbons, which may not fully represent the worst-case compounds in the Stoddard solvent.

C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category

- OECD 2012
  - Because Stoddard solvent is a substance of unknown or variable composition (UVCB), biodegradation results for each constituent characterize the biodegradability of the mixture. There are no biodegradation data specifically for Stoddard solvent. It is a mixture containing n-paraffins (n-alkanes), iso-paraffins (isoalkanes), cyclic-paraffins or naphthenic (cyclics), and aromatics. n-Paraffin constituents are readily biodegradable, but iso-paraffin constituents are only moderately biodegradable (approximately 41% over 41 days). A C9-C13 mixture of aliphatics and aromatics (CAS# 64742-82-1) achieved 75% biodegradation

in 28 days and was classified as readily biodegradable in a test according to OECD Guideline 301F (no additional details were provided).

- Based on the weight of evidence, a score of Very Low was assigned. A compositionally similar member of OECD's C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category was readily biodegradable, and modeling predicts that Stoddard solvent will predict primarily to water and is readily biodegradable. Confidence in this score is reduced because it is based on partially on modeling and because it is unclear whether the biodegradation potential of hydrocarbon solvent of unknown or variable composition may vary greatly depending on the exact constituents present in the mixture.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vH*
Stoddard solvent was assigned a score of Very High for bioaccumulation based on modeled BCF values of up to 11,430 for the surrogate. GreenScreen® criteria classify chemicals as a Very High hazard for bioaccumulation when the BCF/BAF is greater than 5,000 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Environmental Canada – DSL substances that are bioaccumulative

Stoddard solvent (CAS# 8052-41-3)

- U.S. EPA 2012
  - BCFBAF predicts a BAF of 939.2 based on a log K_{ow} of 5.01, indicating this chemical has Moderate bioaccumulation potential because the BAF is between 500 and 1,000 based on a log K_{ow} greater than 5. ToxServices noted that the default structure associated with this CAS number is a straight chain carbohydrate containing 10 carbons, which may not fully represent the worst-case compounds in the Stoddard solvent.

C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category

- OECD 2012
  - Category members have the potential to bioaccumulate based on calculated BCF values ranging from 142 to 11,430 for constituents.
- Based on the weight of evidence, a score of Moderate was assigned. No rationale was provided for the classification of bioaccumulative on Environment Canada's DSL (OECD 2014), and no measured bioaccumulation data are available for Stoddard solvent or other members of OECD's C9-C14 Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category, but calculated BCF values for constituents of these mixtures range from 142 to 11,430. Modeling predicts a BAF of 939.2 for the Stoddard solvent mixture, but the structure modeled may not represent the chemical components that have the highest bioaccumulation potential. Therefore a conservative score of Very High was assigned. Confidence in this score is reduced because it is based on modeling.

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): H
Isopropanol was assigned a score of High for flammability based on classification to DOT class 3 group 2. GreenScreen® criteria classify chemicals as a high hazard for flammability when classified to DOT class 3 group 2 (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* US DOT – Class 3 Group II - flammable liquid
    - *Screening:* Canada WHMIS – Class B3 – combustible liquid
    - *Screening:* GHS-New Zealand – 3.1C (Category 3)– flammable liquid: medium hazard

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 Stoddard Solvent (CAS# 8052-41-3)

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/Genotoxicit	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	**Stoddard solvent**	**8052-41-3**	H	H	DG	DG	DG	DG	DG	M	DG	DG	DG	DG	DG	DG	**H**	**H**	*vL*	*vH*	DG	H

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Stoddard solvent	1

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

Table 6

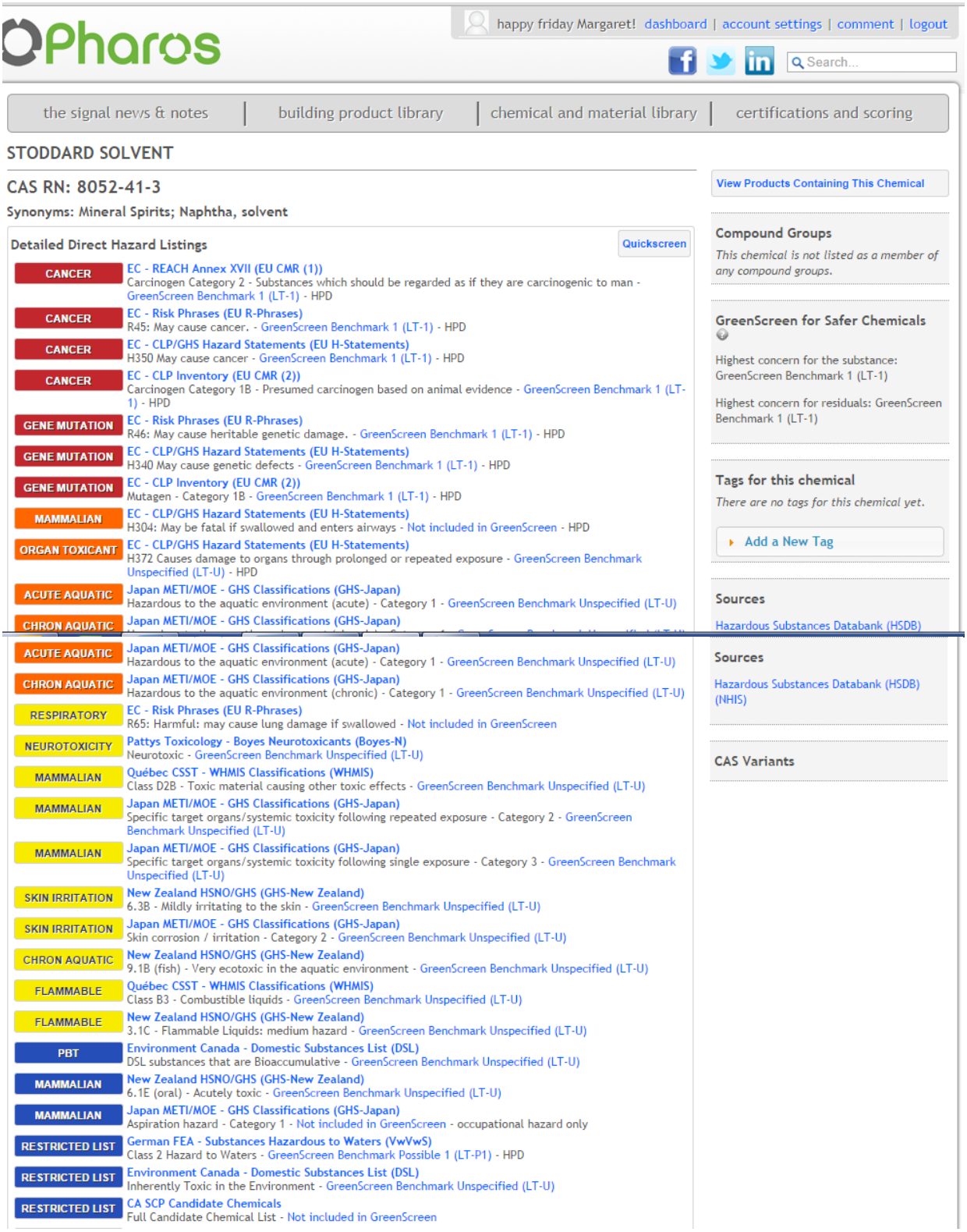
Chemical Name	Final GreenScreen® Benchmark Score
Stoddard solvent	1

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 Stoddard Solvent (CAS# 8052-41-3)



Pharos

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STODDARD SOLVENT

CAS RN: 8052-41-3

Synonyms: Mineral Spirits; Naphtha, solvent

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
ORGAN TOXICANT	EC - CLP/GHS Hazard Statements (EU H-Statements) H372 Causes damage to organs through prolonged or repeated exposure - GreenScreen Benchmark Unspecified (LT-U) - HPD
ACUTE AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan) Hazardous to the aquatic environment (acute) - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan)
ACUTE AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan) Hazardous to the aquatic environment (acute) - Category 1 - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	Japan METI/MOE - GHS Classifications (GHS-Japan) Hazardous to the aquatic environment (chronic) - 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
NEUROTOXICITY	Pattys Toxicology - Boyes Neurotoxicants (Boyes-N) Neurotoxic - GreenScreen Benchmark Unspecified (LT-U)
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) Specific target organs/systemic toxicity following repeated exposure - Category 2 - 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	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 2 - 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)
FLAMMABLE	Québec CSST - WHMIS Classifications (WHMIS) Class B3 - Combustible liquids - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	New Zealand HSNO/GHS (GHS-New Zealand) 3.1C - Flammable Liquids: medium hazard - GreenScreen Benchmark Unspecified (LT-U)
PBT	Environment Canada - Domestic Substances List (DSL) DSL substances that are Bioaccumulative - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	New Zealand HSNO/GHS (GHS-New Zealand) 6.1E (oral) - Acutely toxic - 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	German FEA - Substances Hazardous to Waters (VwVwS) Class 2 Hazard to Waters - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
RESTRICTED LIST	Environment Canada - Domestic Substances List (DSL) Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	CA SCP Candidate Chemicals Full Candidate Chemical List - Not included in GreenScreen

View Products Containing This Chemical

Compound Groups

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

GreenScreen for Safer Chemicals

Highest concern for the substance: GreenScreen Benchmark 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

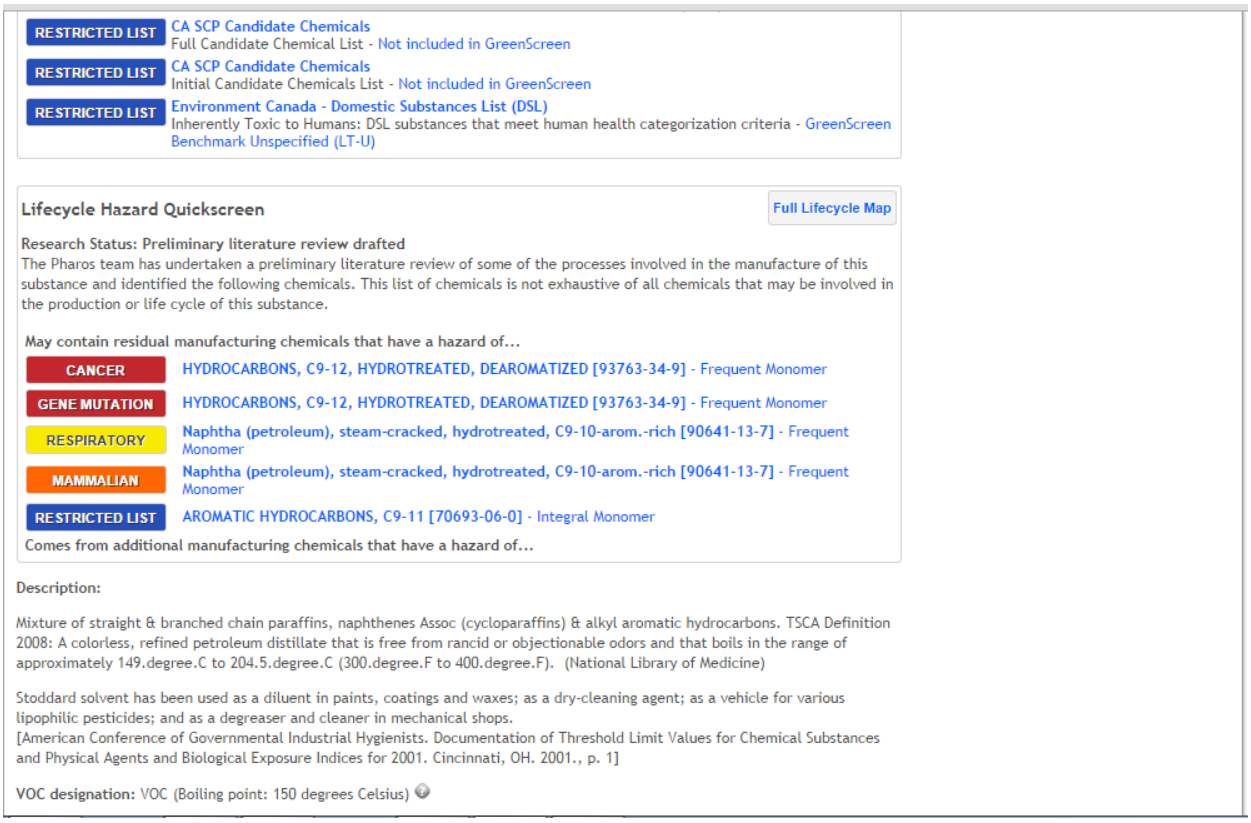
Sources

Hazardous Substances Databank (HSDB)

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants



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

RESTRICTED LIST CA SCP Candidate Chemicals
Initial Candidate Chemicals List - Not included in GreenScreen

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)

Lifecycle Hazard Quickscreen Full Lifecycle Map

Research Status: Preliminary literature review drafted
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...

CANCER HYDROCARBONS, C9-12, HYDROTREATED, DEAROMATIZED [93763-34-9] - Frequent Monomer

GENE MUTATION HYDROCARBONS, C9-12, HYDROTREATED, DEAROMATIZED [93763-34-9] - Frequent Monomer

RESPIRATORY Naphtha (petroleum), steam-cracked, hydrotreated, C9-10-arom.-rich [90641-13-7] - Frequent Monomer

MAMMALIAN Naphtha (petroleum), steam-cracked, hydrotreated, C9-10-arom.-rich [90641-13-7] - Frequent Monomer

RESTRICTED LIST AROMATIC HYDROCARBONS, C9-11 [70693-06-0] - Integral Monomer

Comes from additional manufacturing chemicals that have a hazard of...

Description:

Mixture of straight & branched chain paraffins, naphthenes Assoc (cycloparaffins) & alkyl aromatic hydrocarbons. TSCA Definition 2008: A colorless, refined petroleum distillate that is free from rancid or objectionable odors and that boils in the range of approximately 149.degree.C to 204.5.degree.C (300.degree.F to 400.degree.F). (National Library of Medicine)

Stoddard solvent has been used as a diluent in paints, coatings and waxes; as a dry-cleaning agent; as a vehicle for various lipophilic pesticides; and as a degreaser and cleaner in mechanical shops.
[American Conference of Governmental Industrial Hygienists. Documentation of Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices for 2001. Cincinnati, OH. 2001., p. 1]

VOC designation: VOC (Boiling point: 150 degrees Celsius)

APPENDIX D: EPISuite Modeling Results for Stoddard Solvent (CAS #8052-41-3)

CAS Number: 8052-41-3
SMILES : CCCCCCCCCC
CHEM : Stoddard solvent
MOL FOR: C10 H22
MOL WT : 142.29
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (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 Kow (KowWIN v1.68 estimate) = 5.25
Log Kow (Exper. database match) = 5.01
Exper. Ref: COATES, M. ET AL. (1985)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 164.60 (Adapted Stein & Brown method)
Melting Pt (deg C): -44.13 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 1.73 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C) : 231 (Mean VP of Antoine & Grain methods)
MP (exp database): -29.7 deg C
BP (exp database): 174.1 deg C
VP (exp database): 1.43E+00 mm Hg (1.91E+002 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKow v1.42):
Water Solubility at 25 deg C (mg/L): 1.252
log Kow used: 5.01 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 0.052 mg/L (25 deg C)
Exper. Ref: YALKOWSKY, S.H. & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.091706 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 5.30E+000 atm-m^3/mole (5.37E+005 Pa-m^3/mole)
Group Method: 6.74E+000 atm-m^3/mole (6.83E+005 Pa-m^3/mole)
Exper Database: 5.15E+00 atm-m^3/mole (5.22E+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: 2.587E-001 atm-m^3/mole (2.621E+004 Pa-m^3/mole)
VP: 1.73 mm Hg (source: MPBPVP)
WS: 1.25 mg/L (source: WSKowWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KoaWIN v1.10]:
Log Kow used: 5.01(exp database)
Log Kaw used: 2.323 (exp database)
Log Koa (KoaWIN v1.10 estimate): 2.687
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.8967
Biowin2 (Non-Linear Model): 0.9908
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.4814 (days-weeks)
Biowin4 (Primary Survey Model): 4.1806 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.6850
Biowin6 (MITI Non-Linear Model): 0.8691
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.2494
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days) : 0.9377
BioHC Half-Life (days) : 8.6627

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 191 Pa (1.43 mm Hg)
Log Koa (Koawin est): 2.687
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model : 1.57E-008
Octanol/air (Koa) model: 1.19E-010
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 5.68E-007
Mackay model : 1.26E-006
Octanol/air (Koa) model: 9.55E-009

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 11.1105 E-12 cm^3/molecule-sec
Half-Life = 0.963 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 11.552 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
9.14E-007 (Junge-Pankow, Mackay avg)

9.55E-009 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KocWIN v2.00):
Koc : 1451 L/kg (MCI method)
Log Koc: 3.162 (MCI method)
Koc : 2.227E+004 L/kg (Kow method)
Log Koc: 4.348 (Kow 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 = 1.598 (BCF = 39.66 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.3898 days (HL = 2.454 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.959 (BCF = 910.9)
Log BAF Arnot-Gobas method (upper trophic) = 2.973 (BAF = 939.2)
log Kow used: 5.01 (expkow database)

Volatilization from Water:
Henry LC: 5.15 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 1.217 hours
Half-Life from Model Lake : 113.3 hours (4.721 days)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 99.99 percent
Total biodegradation: 62.01 percent
Total sludge adsorption: 19.73 percent
Total to Air: 18.25 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	26.9	22.1	1000
Water	69.1	208	1000
Soil	1.73	416	1000
Sediment	2.27	1.87e+003	0

Persistence Time: 70.7 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

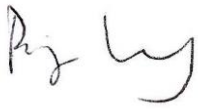
European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

Stoddard solvent GreenScreen® Evaluation Prepared by:

Nikki Maples-Reynolds, MS.
Toxicologist
ToxServices LLC

Stoddard Solvent GreenScreen® Evaluation QC'd by:



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ToxServices LLC