

**Methanol (CAS# 67-56-1) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment**

**Prepared for:**

**Washington State Department of Ecology**

**Prepared by:**

**ToxServices LLC**

**December 1, 2014**



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## GreenScreen® Executive Summary for Methanol (CAS #67-56-1)

Methanol is a chemical that is used as an industrial solvent for inks, resins, adhesives, and dyes, and is also used as antifreeze for automotive radiators, antifreezing agent and octane booster in gasoline, and fuel for picnic stoves.

Methanol 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 developmental toxicity (D) based on classifications on Authoritative A lists in a GreenScreen® list translator search. This corresponds to GreenScreen® benchmark classification 1e in CPA 2011. Additional authoritative A listings were sufficient to assign hazard scores for acute toxicity (AT), systemic toxicity-single dose (STs), 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 methanol 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 Methanol

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*										
NA	NA	NA	<b>H</b>	NA	<b>H</b>	<b>vH</b>	NA	NA	NA	NA	NA	NA	NA	<b>L</b>	<b>L</b>	<b>vL</b>	<b>vL</b>	NA	<b>H</b>

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 Methanol (CAS #67-56-1)

**Method Version: GreenScreen® Version 1.2<sup>1</sup>**  
**Assessment Type<sup>2</sup>: Certified**

**Chemical Name:** Methanol

**CAS Number:** 67-56-1

**GreenScreen® Assessment Prepared By:**

Name: Jennifer Rutkiewicz, Ph.D.

Title: Toxicologist

Organization: ToxServices LLC

Date: July 28, 2014

Assessor Type: Licensed GreenScreen® Profiler

**Quality Control Performed By:**

Name: Bingxuan Wang, Ph.D.

Title: Toxicologist

Organization: ToxServices LLC

Date: December 1, 2014

**Confirm application of the *de minimus* rule<sup>3</sup>:** N/A

**Chemical Structure(s):**



(ChemIDplus 2014)

**Also called:** Methyl alcohol; Alcohol, methyl; Monohydroxymethane (ChemIDplus 2014)

**Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:**

No surrogates were used as methanol is an LT-1 chemical.

**Identify Applications/Functional Uses:** (U.S. EPA 2000)

1. Solvent for inks, resins, adhesives, and dyes
2. Antifreeze for automotive radiators
3. Antifreeze in gasoline
4. Octane booster in gasoline
5. Fuel for picnic stoves

**GreenScreen® Summary Rating for Methanol<sup>4</sup>:** Methanol 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 developmental toxicity (D) based on classifications on Authoritative A lists in a GreenScreen® list translator search. This

<sup>1</sup> Use GreenScreen® Assessment Procedure (Guidance) V1.2

<sup>2</sup> 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)

<sup>3</sup> 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

<sup>4</sup> 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.

corresponds to GreenScreen® benchmark classification 1e in CPA 2011, 2012a. Additional authoritative A listings were sufficient to assign hazard scores for acute toxicity (AT), systemic toxicity-single dose (STs), 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 Methanol did not identify any additional Benchmark 1 score combinations.

**Figure 1: GreenScreen® Hazard Ratings for Methanol**

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*										
NA	NA	NA	<b>H</b>	NA	<b>H</b>	<b>vH</b>	NA	NA	NA	NA	NA	NA	NA	<b>L</b>	<b>L</b>	<b>vL</b>	<b>vL</b>	NA	<b>H</b>

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II\* Human Health endpoints in that they have four hazard scores (i.e. vH, H, M, and L) instead of three (i.e. H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

**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**<sup>5</sup>

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

**Introduction**

Methanol is a chemical that is used as an industrial solvent for inks, resins, adhesives, and dyes, and is also used as antifreeze for automotive radiators, antifreezing agent and octane booster in gasoline, and fuel for picnic stoves (U.S. EPA 2000).

ToxServices assessed methanol 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

<sup>5</sup> 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.

(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 methanol can be found in Appendix C and a summary of the results can be found below:

- Reproductive and Developmental Toxicity
  - US NIH - Reproductive & Developmental Monographs (NTP-OHAaT) A-Clear evidence of adverse developmental toxicant effects
  - Cal/EPA - Chemicals Known to Cause Cancer & Reproductive Toxicity (Prop 65) Developmental toxicity
  - German MAK - List of Substances (MAK) Pregnancy Risk Group C
  - US NIH - Reproductive & Developmental Monographs (NTP-OHAaT) D-Insufficient evidence for a conclusion on adverse reproductive toxicant effects
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 1B
  - New Zealand HSNO/GHS (GHS-New Zealand): 6.8B - Suspected human reproductive or developmental toxicants
- Mammalian Toxicity
  - EC - CLP/GHS Hazard Statements (EU H-Statements) H301 Toxic if swallowed
  - EC - CLP/GHS Hazard Statements (EU H-Statements): H311 Toxic in contact with skin
  - EC - CLP/GHS Hazard Statements (EU H-Statements) H331 Toxic if inhaled
  - EC - Risk Phrases (EU R-Phrases): R23/24/25: Toxic by inhalation, in contact with skin, and if swallowed
  - Québec CSST - WHMIS Classifications (WHMIS) Class D1B - Toxic material causing immediate and serious toxic effects
  - New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (dermal) - Acutely toxic
  - New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (inhalation)
  - New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (oral)
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (oral) - Category 5
  - Québec CSST - WHMIS Classifications (WHMIS) Class D2A - Very toxic material causing other toxic effects
  - EC - Risk Phrases (EU R-Phrases) R39/23/24/25: Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed
  - EC - CLP/GHS Hazard Statements (EU H-Statements) H370 Causes damage to organs
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 1
  - New Zealand HSNO/GHS (GHS-New Zealand) 6.9A (inhalation) - Toxic to human target organs or systems
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following repeated exposure - Category 1
- Neurotoxicity
  - Lancet - Grandjean and Landrigan Neurotoxic Chemicals (G&L Neuro) Known to be neurotoxic in man (Grandjean and Landrigan 2006, 2014).
- Eye Irritation
  - New Zealand HSNO/GHS (GHS-New Zealand) 6.4A - Irritating to the eye
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2

- Persistence
  - Environment Canada - Domestic Substances List (DSL) DSL substances that are Persistent
- Flammability
  - U.S. DOT Hazard Class 3, Packing Group II
  - EC - CLP/GHS Hazard Statements (EU H-Statements) H225 Highly flammable liquid and vapor
  - EC - Risk Phrases (EU R-Phrases) R11: Highly flammable liquid
  - Québec CSST - WHMIS Classifications (WHMIS) Class B2 - Flammable liquids
  - New Zealand HSNO/GHS (GHS-New Zealand) 3.1B - Flammable Liquids: high hazard
  - Japan METI/MOE - GHS Classifications (GHS-Japan) Flammable liquids - Category 2
- Other
  - German FEA - Substances Hazardous to Waters (VwVwS) Class 1 Low Hazard to Waters
  - Environment Canada - Domestic Substances List (DSL) Inherently Toxic to Humans: DSL substances that meet human health categorization criteria

**PhysicoChemical Properties of Methanol**

Methanol is a colorless liquid at room temperature. Its high vapor pressure of 127 mmHg indicates that it is likely to form a gas at room temperature. It is highly soluble in water and its log K<sub>ow</sub> of -0.77 indicates low potential for bioaccumulation.

<b>Table 1: Physical and Chemical Properties of Methanol (CAS #67-56-1)</b>		
<b>Property</b>	<b>Value</b>	<b>Reference</b>
Molecular formula	CH <sub>4</sub> O	ChemIDplus 2014
SMILES Notation	CO	ChemIDplus 2014
Molecular weight	32.04	ChemIDplus 2014
Physical state	Liquid	ECHA 2014
Appearance	Colorless	ECHA 2014
Melting point	-97.6°C	ChemIDplus 2014
Vapor pressure	127 mmHg at 25°C	ChemIDplus 2014
Water solubility	1 x 10 <sup>6</sup> mg/L at 25°C	ChemIDplus 2014
Dissociation constant	pKa = 15.3	ChemIDplus 2014
Density/specific gravity	0.79-0.7 at 20°C	ECHA 2014
Partition coefficient	log K <sub>ow</sub> = -0.77	ChemIDplus 2014

**Hazard Classification Summary Section:**

**Group I Human Health Effects (Group I Human)**

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

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

### **Mutagenicity/Genotoxicity (M) 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

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

- Authoritative and Screening Lists
  - *Authoritative:* US NIH - Reproductive & Developmental Monographs (NTP-OHAaT) D- Insufficient evidence for a conclusion on adverse reproductive toxicant effects
  - *Screening:* Not present on any screening lists

### **Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): H**

Methanol was assigned a score of High for developmental toxicity based on presence on authoritative lists. GreenScreen<sup>®</sup> criteria classify chemicals as a High hazard for developmental toxicity when listed as a developmental toxicant on the California EPA's Proposition 65 list and as having Clear Evidence of Adverse Effects – Developmental by NTP-OHAaT (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* US NIH - Reproductive & Developmental Monographs (NTP-OHAaT) A- Clear evidence of adverse developmental toxicant effects
  - *Authoritative:* Cal/EPA - Chemicals Known to Cause Cancer & Reproductive Toxicity (Prop 65) Developmental toxicity
  - *Authoritative:* German MAK - List of Substances (MAK) Pregnancy Risk Group C
  - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 1B
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 6.8B - Suspected human reproductive or developmental toxicants

### **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
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- High Throughput Screening (HTS) Data –
  - HTS data were identified for methanol using PubChem (<http://pubchem.ncbi.nlm.nih.gov/>).
  - The data included the following results:
    - Methanol was active in 0/7 androgen receptor agonist assays and 0/13 androgen receptor antagonist assays.
    - Methanol was active in 0/7 estrogen receptor-alpha agonist assays and 0/13 estrogen receptor-alpha antagonist assays.
    - Methanol was active in 0/3 thyroid receptor agonist assays and 0/7 thyroid receptor antagonist assays.
    - Methanol was active in 0/2 thyroid stimulating hormone receptor agonist assays. No data were available for thyroid stimulating hormone receptor antagonist assays.
- 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): H**

Methanol was assigned a score of High for acute toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a High hazard for acute toxicity when associated with the EU H-statements H301: Toxic if swallowed, H311: Toxic in contact with skin, and H331: Toxic if inhaled (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements) H301 Toxic if swallowed
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements): H311 Toxic in contact with skin
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements) H331 Toxic if inhaled
  - *Authoritative:* EC - Risk Phrases (EU R-Phrases): R23/24/25: Toxic by inhalation, in contact with skin, and if swallowed
  - *Screening:* Québec CSST - WHMIS Classifications (WHMIS) Class D1B - Toxic material causing immediate and serious toxic effects
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (oral) - Acutely toxic
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (dermal) - Acutely toxic
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.1C (inhalation) - Acutely toxic
  - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (oral) - Category 5

#### **Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)**

##### **Group II Score (single dose) (vH, H, M, or L): vH**

Methanol was assigned a score of Very High for systemic toxicity (single dose) based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Very High hazard for systemic toxicity (single dose) when the chemical is associated with the EU-H-statement H370: Causes damage to organs and EU R-phrase R39/23/24/25 : Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements) H370 Causes damage to organs
  - *Authoritative:* EC - Risk Phrases (EU R-Phrases) R39/23/24/25: Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed
  - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 1
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.9A (inhalation) - Toxic to human target organs or systems

##### **Group II\* Score (repeated dose) (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 repeated exposure - Category 1

### **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:* Lancet - Grandjean and Landrigan Neurotoxic Chemicals (G&L Neuro) Known to be neurotoxic in man

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Lancet - Grandjean and Landrigan Neurotoxic Chemicals (G&L Neuro) Known to be neurotoxic in man

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

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

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

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

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

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

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

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.4A - Irritating to the eye
  - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2

### **Ecotoxicity (Ecotox)**

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

Methanol was assigned a score of Low for acute aquatic toxicity based on measured values all greater than 10,000 mg/L. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute toxicity values are above 100 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: Due to the large number of studies available in the REACH dossier, only those identified as Key studies were summarized.

- 96-hr LC<sub>50</sub> (*Lepomis macrochirus*, bluegill) = 15,400 mg/L
- 96-hr EC<sub>50</sub> (*Daphnia magna*, water flea) = 18,260 mg/L
- 96-hr EC<sub>50</sub> (*Selenastrum capricornutum*, green algae) = 22,000 mg/L

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

Methanol was assigned a score of Low for chronic aquatic toxicity based on modeled values that are greater than 100 mg/L. GreenScreen<sup>®</sup> criteria classify chemicals as a Low hazard for chronic aquatic toxicity when chronic toxicity values are above 10 mg/L (CPA 2012a). There is low confidence in the hazard level, as the values were from modeled data.

- Authoritative and Screening Lists
  - *Authoritative*: Not present on any authoritative lists
  - *Screening*: Not present on any screening lists
- ECHA 2014
  - 200-hr EC<sub>50</sub> (*Oryzias latipes*, killifish) = 9,164-14,536 mg/L
- U.S. EPA 2012a
  - ChV (fish) = 447 mg/L
  - ChV (daphnid) = 134 mg/L
  - ChV (green algae) = 113 mg/L (Appendix D)

### **Environmental Fate (Fate)**

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

Methanol was assigned a score of Very Low for persistence based on numerous studies showing that it is readily biodegradable and meets the ten-day window. GreenScreen<sup>®</sup> criteria classify chemicals as a Very Low hazard for persistence when meeting the ten-day window in ready biodegradation studies (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative*: Not present on any authoritative lists
  - *Screening*: Environment Canada - Domestic Substances List (DSL) DSL substances that are Persistent
- ECHA 2014
  - In a ready biodegradation study (GLP-compliance and guideline not indicated) according to domestic non-activated sludge inoculum, methanol (3-10 mg/L starting concentration) achieved 95% biodegradation in 20 days, with 88% biodegradation occurring in 10 days. Authors concluded that the substance is readily biodegradable and meeting the 10-day biodegradation window.
- U.S. EPA 2014
  - In a ready biodegradation study (GLP-compliance and guideline not indicated) according to adapted activated sludge inoculum, methanol (starting concentration not known) achieved 50-80% biodegradation in six days. Authors concluded that the substance is readily biodegradable.
  - In a ready biodegradation study (GLP-compliance and guideline not indicated) according to domestic sewage inoculum under anaerobic conditions, methanol (starting concentration not known) achieved >50% biodegradation in seven hours. Methanol is rapidly biodegraded under anaerobic conditions by sediment and groundwater polluted by municipal landfill leachate.

- U.S. EPA 2012b
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that methanol expected to be readily biodegradable. Fugacity modeling predicts 50.4% will partition to soil with a half-life of 17 days, 39.3% will partition to water with a half-life of 9 days, and 10.3% will partition to air with a half-life of 11 days (Appendix E).

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

Methanol was assigned a score of Very Low for bioaccumulation based on BCF less than 10.

GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when BCF values are less than 100 (CPA 2012a). There is low confidence in the hazard level, as the studies were not well-characterized.

- Authoritative and Screening Lists
  - *Authoritative*: Not present on any authoritative lists
  - *Screening*: Not present on any screening lists
- U.S. EPA 2012b
  - BCFBAF predicts a BCF of 3.2 based on a log  $K_{ow}$  of -0.63, indicating this chemical is not likely to bioaccumulate because the BCF is less than 100 based on a log  $K_{ow}$  less than 5.
- HSDB 2012
  - A BCF < 10 has been measured in golden ide exposed to 0.05 mg/L methanol for 3 days. No additional details were provided.

**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**

Methanol was assigned a score of High for flammability based on presence on authoritative lists.

GreenScreen® criteria classify chemicals as a High hazard for flammability when the chemical is associated with the EU H-Statement H225:H highly flammable liquid and vapor (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative*: U.S. DOT Hazard Class 3, Packing Group II
  - *Authoritative*: EC - CLP/GHS Hazard Statements (EU H-Statements) H225 Highly flammable liquid and vapor
  - *Authoritative*: EC - Risk Phrases (EU R-Phrases) R11: Highly flammable liquid
  - *Screening*: Québec CSST - WHMIS Classifications (WHMIS) Class B2 - Flammable liquids
  - *Screening*: New Zealand HSNO/GHS (GHS-New Zealand) 3.1B - Flammable Liquids: high hazard
  - *Screening*: Japan METI/MOE - GHS Classifications (GHS-Japan) Flammable liquids - Category 2

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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 Methanol (CAS #67-56-1)**

 			GreenScreen® Score Inspector																					
			Table 1: Hazard Table			Group I Human										Group II and II* Human						Ecotox		Fate
Inorganic Chemical?	Chemical Name	CAS#	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				
			S	R*	S	R*	*	*	AA	CA	P	B	Rx	F										
No	Methanol	67-56-1	DG	DG	DG	H	DG	H	vH	DG	DG	DG	DG	DG	DG	DG	L	L	vL	vL	DG	H		

  

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
Methanol	1
Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score	

Table 6	
Chemical Name	Final GreenScreen® Benchmark Score
Methanol	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 Methanol (CAS #67-56-1)

happy wednesday Margaret! [dashboard](#) | [a](#) [statement](#)[f](#) [t](#) [in](#)

[the signal news & notes](#) | [building product library](#) | [chemical and material library](#) | [certifications and scoring](#)

### METHANOL

**CAS RN: 67-56-1**  
Synonyms: Methyl alcohol

[View Products Containing This Chemical](#)

**Detailed Direct Hazard Listings** [Quickscreen](#)

<b>DEVELOPMENTAL</b>	<a href="#">US NIH - Reproductive &amp; Developmental Monographs (NTP-OHAaT)</a> A-Clear evidence of adverse developmental toxicant effects - <a href="#">GreenScreen Benchmark 1 (LT-1)</a> - HPD
<b>DEVELOPMENTAL</b>	<a href="#">Cal/EPA - Chemicals Known to Cause Cancer &amp; Reproductive Toxicity (Prop 65)</a> Developmental toxicity - <a href="#">GreenScreen Benchmark 1 (LT-1)</a> - HPD
<b>REPRODUCTIVE</b>	<a href="#">Japan METI/MOE - GHS Classifications (GHS-Japan)</a> Toxic to reproduction - Category 1B - <a href="#">GreenScreen Benchmark Possible 1 (LT-P1)</a>
<b>REPRODUCTIVE</b>	<a href="#">New Zealand HSNO/GHS (GHS-New Zealand)</a> 6.8B - Suspected human reproductive or developmental toxicants - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>MAMMALIAN</b>	<a href="#">EC - CLP/GHS Hazard Statements (EU H-Statements)</a> H311 Toxic in contact with skin - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a> - HPD
<b>MAMMALIAN</b>	<a href="#">Japan METI/MOE - GHS Classifications (GHS-Japan)</a> Specific target organs/systemic toxicity following repeated exposure - Category 1 - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>MAMMALIAN</b>	<a href="#">Japan METI/MOE - GHS Classifications (GHS-Japan)</a> Specific target organs/systemic toxicity following single exposure - Category 1 - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>ORGAN TOXICANT</b>	<a href="#">EC - Risk Phrases (EU R-Phrases)</a> R39: Danger of very serious irreversible effects. - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a> - HPD
<b>ORGAN TOXICANT</b>	<a href="#">EC - CLP/GHS Hazard Statements (EU H-Statements)</a> H370 Causes damage to organs - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a> - HPD
<b>ORGAN TOXICANT</b>	<a href="#">New Zealand HSNO/GHS (GHS-New Zealand)</a> 6.9A (inhalation) - Toxic to human target organs or systems - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>FLAMMABLE</b>	<a href="#">EC - CLP/GHS Hazard Statements (EU H-Statements)</a> H225 Highly flammable liquid and vapour. - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a> - occupational hazard only - HPD
<b>FLAMMABLE</b>	<a href="#">New Zealand HSNO/GHS (GHS-New Zealand)</a> 3.1B - Flammable Liquids: high hazard - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>FLAMMABLE</b>	<a href="#">Japan METI/MOE - GHS Classifications (GHS-Japan)</a> Flammable liquids - Category 2 - <a href="#">GreenScreen Benchmark Unspecified (LT-U)</a>
<b>FLAMMABLE</b>	<a href="#">EC - Risk Phrases (EU R-Phrases)</a>

**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 \(HSDB\) \(NHIS\)](#)

**CAS Variants**

<b>FLAMMABLE</b>	<b>EC - Risk Phrases (EU R-Phrases)</b> R11: Highly flammable LIQUID - Not included in GreenScreen
<b>DEVELOPMENTAL</b>	<b>German MAK - List of Substances (MAK)</b> Pregnancy Risk Group C - GreenScreen Benchmark Unspecified (LT-U)
<b>REPRODUCTIVE</b>	<b>US NIH - Reproductive &amp; Developmental Monographs (NTP-OHAaT)</b> D-Insufficient evidence for a conclusion on adverse reproductive toxicant effects - GreenScreen Benchmark Unspecified (LT-U)
<b>NEUROTOXICITY</b>	<b>Lancet - Grandjean &amp; Landrigan Neurotoxic Chemicals (G&amp;L Neuro)</b> Known to be neurotoxic in man - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>EC - Risk Phrases (EU R-Phrases)</b> R23: Toxic by inhalation. - GreenScreen Benchmark Unspecified (LT-U) - HPD
<b>MAMMALIAN</b>	<b>EC - Risk Phrases (EU R-Phrases)</b> R24: Toxic in contact with skin. - GreenScreen Benchmark Unspecified (LT-U) - HPD
<b>MAMMALIAN</b>	<b>EC - Risk Phrases (EU R-Phrases)</b> R25: Toxic if swallowed. - GreenScreen Benchmark Unspecified (LT-U) - HPD
<b>MAMMALIAN</b>	<b>EC - CLP/GHS Hazard Statements (EU H-Statements)</b> H301 Toxic if swallowed - GreenScreen Benchmark Unspecified (LT-U) - HPD
<b>MAMMALIAN</b>	<b>EC - CLP/GHS Hazard Statements (EU H-Statements)</b> H331 Toxic if inhaled - GreenScreen Benchmark Unspecified (LT-U) - HPD
<b>MAMMALIAN</b>	<b>Québec CSST - WHMIS Classifications (WHMIS)</b> Class D1B - Toxic material causing immediate and serious toxic effects - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>Québec CSST - WHMIS Classifications (WHMIS)</b> Class D2A - Very toxic material causing other toxic effects - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>Québec CSST - WHMIS Classifications (WHMIS)</b> Class D2B - Toxic material causing other toxic effects - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>New Zealand HSNO/GHS (GHS-New Zealand)</b> 6.1C (dermal) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>New Zealand HSNO/GHS (GHS-New Zealand)</b> 6.1C (inhalation) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>New Zealand HSNO/GHS (GHS-New Zealand)</b> 6.1C (oral) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
<b>MAMMALIAN</b>	<b>Japan METI/MOE - GHS Classifications (GHS-Japan)</b> Acute toxicity (oral) - Category 5 - GreenScreen Benchmark Unspecified (LT-U)
<b>EYE IRRITATION</b>	<b>New Zealand HSNO/GHS (GHS-New Zealand)</b> 6.4A - Irritating to the eye - GreenScreen Benchmark Unspecified (LT-U)
<b>EYE IRRITATION</b>	<b>Japan METI/MOE - GHS Classifications (GHS-Japan)</b> Serious eye damage / eye irritation - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
<b>TERRESTRIAL</b>	<b>New Zealand HSNO/GHS (GHS-New Zealand)</b> 9.3C - Harmful to terrestrial vertebrates - Not included in GreenScreen
<b>FLAMMABLE</b>	<b>Québec CSST - WHMIS Classifications (WHMIS)</b> Class B2 - Flammable liquids - GreenScreen Benchmark Unspecified (LT-U)
<b>PBT</b>	<b>Environment Canada - Domestic Substances List (DSL)</b> DSL substances that are Persistent - GreenScreen Benchmark Unspecified (LT-U)
<b>RESTRICTED LIST</b>	<b>US EPA - Hazardous Air Pollutants (HAPs)</b> Hazardous Air Pollutant subject to the Clean Air Act - Not included in GreenScreen

statement

<b>PBT</b>	Environment Canada - Domestic Substances List (DSL) DSL substances that are Persistent - GreenScreen Benchmark Unspecified (LT-U)
<b>RESTRICTED LIST</b>	US EPA - Hazardous Air Pollutants (HAPs) Hazardous Air Pollutant subject to the Clean Air Act - Not included in GreenScreen
<b>RESTRICTED LIST</b>	German FEA - Substances Hazardous to Waters (VwVwS) Class 1 Low Hazard to Waters - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only
<b>RESTRICTED LIST</b>	CA SCP Candidate Chemicals Full Candidate Chemical List - Not included in GreenScreen
<b>RESTRICTED LIST</b>	CA SCP Candidate Chemicals Initial Candidate Chemicals List - Not included in GreenScreen

statement

**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...

<b>CANCER</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>GENE MUTATION</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>RESPIRATORY</b>	ZINC OXIDE [1314-13-2] - Frequent Catalyst
<b>MAMMALIAN</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>EYE IRRITATION</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>SKIN SENSITIZE</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>ACUTE AQUATIC</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>CHRON AQUATIC</b>	ZINC OXIDE [1314-13-2] - Frequent Catalyst
<b>TERRESTRIAL</b>	COPPER [7440-50-8] - Frequent Catalyst
<b>RESTRICTED LIST</b>	COPPER [7440-50-8] - Frequent Catalyst

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

<b>PBT</b>	HYDROGEN [1333-74-0] - Integral Feedstock
<b>DEVELOPMENTAL</b>	CARBON MONOXIDE [630-08-0] - Integral Feedstock
<b>REPRODUCTIVE</b>	CARBON MONOXIDE [630-08-0] - Integral Feedstock
<b>NEUROTOXICITY</b>	CARBON MONOXIDE [630-08-0] - Integral Feedstock
<b>ORGAN TOXICANT</b>	CARBON MONOXIDE [630-08-0] - Integral Feedstock
<b>FLAMMABLE</b>	HYDROGEN [1333-74-0] - Integral Feedstock
<b>REACTIVE</b>	HYDROGEN [1333-74-0] - Integral Feedstock

Description:

Product name:  CAS#

There is no information in ESIS for this substance with respect to the BPD.

**Classification and Labelling Information:**

Annex I Index# : 603-001-00-X  
 Substance Name : methanol  
 in Annex 1  
 Note : Not available  
 ATP : 

Inserted	Updated
CLP00	-

Classification : F; R11 - T; R23/24/25-39/23/24/25  
 Risk Phrases : + R11 : [Highly flammable.](#)  
 : + R23/24/25 : [Toxic by inhalation, in contact with skin and if swallowed.](#)  
 : + R39/23/24/25 : [Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.](#)

Safety Phrases : + S1/2 : [Keep locked up and out of the reach of children.](#)  
 : + S7 : [Keep container tightly closed.](#)  
 : + S16 : [Keep away from sources of ignition - No smoking.](#)  
 : + S36/37 : [Wear suitable protective clothing and gloves.](#)  
 : + S45 : [In case of accident or if you feel unwell, seek medical advice immediately \(show the label where possible\).](#)

Symbol(s) and Indication(s) of Danger :  + F :

gas, refrigerated liquid (cryogenic liquid), with high methane content).												
Methanesulfonyl chloride .....	6.1	UN3246	I	6.1, 8	2, B9, B14, B32, B74, T20, TP2, TP12, TP13, TP38, TP45	None	227	244	Forbidden	Forbidden	D	40
Methanol .....	3	UN1230	II	3, 6.1	IB2, T7, TP2	150	202	242	1 L	60 L	B	40
Methanol .....	3	UN1230	II	3	IB2, T7, TP2	150	202	242	1 L	60 L	B	40
Methazoic acid .....	Forbidden											
4-Methoxy-4-methylpentan-2-one.	3	UN2293	III	3	B1, IB3, T2, TP1	150	203	242	60 L	220 L	A	
1-Methoxy-2-propanol .....	3	UN3092	III	3	B1, IB3, T2, TP1	150	203	242	60 L	220 L	A	
Methoxymethyl isocyanate .....	3	UN2605	I	3, 6.1	1, B9, B14, B30, B72, T22, TP2, TP13, TP38, TP44	None	226	244	Forbidden	Forbidden	D	40
Methyl acetate .....	3	UN1231	II	3	IB2, T4, TP1	150	202	242	5 L	60 L	B	

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

ECOSAR Version 1.11 Results Page

SMILES: OC  
 CHEM: Methanol  
 CAS Num: 000067-56-1  
 ChemID1:  
 MOL FOR: C1 H4 O1  
 MOL WT: 32.04  
 Log K<sub>ow</sub>: -0.632 (EPISuite K<sub>ow</sub>win v1.68 Estimate)  
 Log K<sub>ow</sub>: (User Entered)  
 Log K<sub>ow</sub>: -0.77 (PhysProp DB exp value - for comparison only)  
 Melt Pt: (User Entered for Wat Sol estimate)  
 Melt Pt: -97.60 (deg C, PhysProp DB exp value for Wat Sol est)  
 Wat Sol: 1E+006 (mg/L, EPISuite WSK<sub>ow</sub>win v1.43 Estimate)  
 Wat Sol: (User Entered)  
 Wat Sol: 1E+006 (mg/L, PhysProp DB exp value)

-----  
 Values used to Generate ECOSAR Profile  
 -----

Log K<sub>ow</sub>: -0.632 (EPISuite K<sub>ow</sub>win v1.68 Estimate)  
 Wat Sol: 1E+006 (mg/L, PhysProp DB exp value)

-----  
 Available Measured Data from ECOSAR Training Set  
 -----

CAS No	Organism	Measured		Ecosar Class	Reference
		Duration	End Pt mg/L (ppm)		
000067-56-1	Fish	96-hr.	LC50 29400	Neutral organics	DUL

-----  
 ECOSAR v1.1 Class-specific Estimations  
 -----

Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr.	LC50	6086.885
Neutral Organics	: Daphnid	48-hr.	LC50	2710.440
Neutral Organics	: Green Algae	96-hr.	EC50	739.102

Neutral Organics	: Fish	ChV	446.670
Neutral Organics	: Daphnid	ChV	134.393
Neutral Organics	: Green Algae	ChV	112.652
Neutral Organics	: Fish (SW)	96-hr. LC50	7543.122
Neutral Organics	: Mysid	96-hr. LC50	33348.301
Neutral Organics	: Fish (SW)	ChV	164.084
Neutral Organics	: Mysid (SW)	ChV	6288.554
Neutral Organics	: Earthworm	14-day LC50	104.447

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

-----  
Class Specific LogK<sub>ow</sub> Cut-Offs  
-----

If the log K<sub>ow</sub> of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:  
-----

Maximum LogK<sub>ow</sub>: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)  
Maximum LogK<sub>ow</sub>: 6.0 (Earthworm LC50)  
Maximum LogK<sub>ow</sub>: 6.4 (Green Algae EC50)  
Maximum LogK<sub>ow</sub>: 8.0 (ChV)

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

CAS Number: 67-56-1

SMILES: OC

CHEM: Methanol

MOL FOR: C1 H4 O1

MOL WT: 32.04

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log  $K_{ow}$  (octanol-water): -0.77  
Boiling Point (deg C): 64.60  
Melting Point (deg C): -97.60  
Vapor Pressure (mm Hg): 127  
Water Solubility (mg/L): 1E+006  
Henry LC (atm-m<sup>3</sup>/mole): 4.55E-006

Log Octanol-Water Partition Coef (SRC):

Log  $K_{ow}$  ( $K_{ow}$ WIN v1.68 estimate) = -0.63  
Log  $K_{ow}$  (Exper. database match) = -0.77  
Exper. Ref: HANSCH, C. ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 39.35 (Adapted Stein & Brown method)  
Melting Pt (deg C): -101.00 (Mean or Weighted MP)  
VP (mm Hg, 25 deg C): 119 (Mean VP of Antoine & Grain methods)  
VP (Pa, 25 deg C): 1.59E+004 (Mean VP of Antoine & Grain methods)  
MP (exp database): -97.6 deg C  
BP (exp database): 64.7 deg C  
VP (exp database): 1.27E+02 mm Hg (1.69E+004 Pa) at 25 deg C

Water Solubility Estimate from Log  $K_{ow}$  (WSK<sub>ow</sub> v1.42):

Water Solubility at 25 deg C (mg/L): 1e+006  
log  $K_{ow}$  used: -0.77 (user entered)  
melt pt used: -97.60 deg C  
Water Sol (Exper. database match) = 1e+006 mg/L (25 deg C)  
Exper. Ref: RIDDICK, J.A. ET AL. (1986)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:  
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method: 4.27E-006 atm-m<sup>3</sup>/mole (4.32E-001 Pa-m<sup>3</sup>/mole)  
Group Method: 3.62E-006 atm-m<sup>3</sup>/mole (3.67E-001 Pa-m<sup>3</sup>/mole)  
Exper Database: 4.55E-06 atm-m<sup>3</sup>/mole (4.61E-001 Pa-m<sup>3</sup>/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: 4.550E-006 atm-m<sup>3</sup>/mole (4.610E-001 Pa-m<sup>3</sup>/mole)  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 5.354E-006 atm-m<sup>3</sup>/mole (5.425E-001 Pa-m<sup>3</sup>/mole)  
VP: 127 mm Hg (source: User-Entered)  
WS: 1E+006 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [K<sub>oa</sub>WIN v1.10]:

Log K<sub>ow</sub> used: -0.77 (user entered)  
Log K<sub>aw</sub> used: -3.730 (user entered)  
Log K<sub>oa</sub> (K<sub>oa</sub>WIN v1.10 estimate): 2.960  
Log K<sub>oa</sub> (experimental database): 2.880

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model): 0.8910  
Biowin2 (Non-Linear Model): 0.9752  
Expert Survey Biodegradation Results:  
Biowin3 (Ultimate Survey Model): 3.2883 (days-weeks)  
Biowin4 (Primary Survey Model): 3.9310 (days)  
MITI Biodegradation Probability:  
Biowin5 (MITI Linear Model): 0.7784  
Biowin6 (MITI Non-Linear Model): 0.9324  
Anaerobic Biodegradation Probability:  
Biowin7 (Anaerobic Linear Model): 0.8893  
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 1.69E+004 Pa (127 mm Hg)  
Log K<sub>oa</sub> (Exp database): 2.880  
Kp (particle/gas partition coef. (m<sup>3</sup>/μg)):  
Mackay model: 1.77E-010  
Octanol/air (K<sub>oa</sub>) model: 1.86E-010  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model: 6.4E-009  
Mackay model: 1.42E-008  
Octanol/air (K<sub>oa</sub>) model: 1.49E-008

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:  
OVERALL OH Rate Constant = 0.6160 E-12 cm<sup>3</sup>/molecule-sec  
Half-Life = 17.364 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
Ozone Reaction:  
No Ozone Reaction Estimation  
Fraction sorbed to airborne particulates (phi):  
1.03E-008 (Junge-Pankow, Mackay avg)  
1.49E-008 (K<sub>oa</sub> method)  
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient ( $K_{oc}$  WIN v2.00):

$K_{oc}$ : 1 L/kg (MCI method)  
Log  $K_{oc}$ : 0.000 (MCI method)  
 $K_{oc}$ : 1.224 L/kg ( $K_{ow}$  method)  
Log  $K_{oc}$ : 0.088 ( $K_{ow}$  method)  
Experimental Log  $K_{oc}$ : 0.44 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 = 0.500 (BCF = 3.162 L/kg wet-wt)  
Log Biotransformation Half-life (HL) = -1.6723 days (HL = 0.02126 days)  
Log BCF Arnot-Gobas method (upper trophic) = -0.045 (BCF = 0.9013)  
Log BAF Arnot-Gobas method (upper trophic) = -0.045 (BAF = 0.9013)  
log  $K_{ow}$  used: -0.77 (user entered)

Volatilization from Water:

Henry LC: 4.55E-006 atm-m<sup>3</sup>/mole (entered by user)  
Half-Life from Model River: 73.41 hours (3.059 days)  
Half-Life from Model Lake: 848.3 hours (35.35 days)

Removal In Wastewater Treatment:

Total removal: 92.07 percent  
Total biodegradation: 91.69 percent  
Total sludge adsorption: 0.33 percent  
Total to Air: 0.04 percent  
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	10.3	272	1000
Water	39.3	208	1000
Soil	50.4	416	1000
Sediment	0.0695	1.87e+003	0

Persistence Time: 261 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**

**Methanol GreenScreen® Evaluation Prepared by:**



Jennifer Rutkiewicz, Ph.D.  
Toxicologist  
ToxServices LLC

**Methanol GreenScreen® Evaluation QC'd by:**



Bingxuan Wang, Ph.D.  
Toxicologist  
ToxServices LLC