Octamethylcyclotetrasiloxane (CAS# 556-67-2) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

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December 1, 2014

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GreenScreen® Executive Summary for Octamethylcyclotetrasiloxane (CAS #556-67-2)

Octamethylcyclotetrasiloxane is commonly referred to as D4. It is a key ingredient in a variety of product formulations (cosmetics and pharmaceuticals) and a critical intermediate in the production of silicone polymers.

Octamethylcyclotetrasiloxane was assigned a GreenScreen® Benchmark Score of 1 ("Avoid-Chemical of High Concern") as it has Very High persistence (P), Very High bioaccumulation (B), and Very High Ecotoxicity (chronic aquatic toxicity (CA)), which corresponds to GreenScreen® benchmark classifications 1a, 1b, 1c and 1d in CPA 2011. As assessment of these endpoints revealed that octamethylcyclotetrasiloxane is a Benchmark 1 chemical, assessment of additional endpoints was not performed. Additional authoritative A listings were sufficient to assign hazard scores for reproductive toxicity (R).

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 Octamethylcyclotetrasiloxane

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

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms. NA: Not assessed.

GreenScreen® Assessment for Octamethylcyclotetrasiloxane (CAS #556-67-2)

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

Chemical Name: Octamethylcyclotetrasiloxane

CAS Number: 556-67-2

GreenScreen® Assessment Prepared By:
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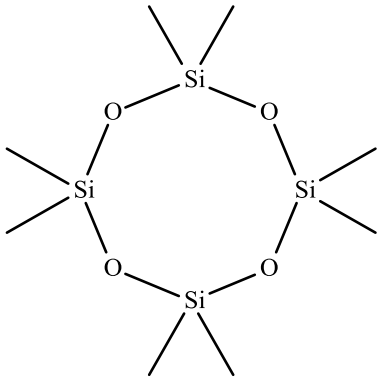
Title: Toxicologist
Organization: ToxServices LLC
Date: August 29, 2014
Assessor Type: Licensed GreenScreen® Profiler

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[3]: N/A

Chemical Structure(s):



CAS #556-67-2

Also called: Cyclic dimethylsiloxane tetramer, Cyclen D4/OMCTS, Cyclen D4/OMCTS WN, Cyclomethicone, Cyclotetrasiloxane, octamethyl-, Cyclotetrasiloxane, D4, Dow Corning 244, KF 994, DC 344, DC 244, Dow Corning 344, NUC silicone VS 7207, Oel Z020, OMCTS, SF 1173, Tetramere D4/OMCTS, Tetramere D4/OMCTS Silbione, TSF 404, Volasil 244 and VS 7207 (ECHA 2014)

[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

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
No surrogates were used as available data on critical endpoints for octamethylcyclotetrasiloxane are sufficient to assign a score of Benchmark 1.

Identify Applications/Functional Uses: (ECHA 2014)
1. Chemical intermediate at the site of production.
2. In personal care products (e.g. cosmetic, skin- and hair-care products).
3. In household products (e.g. cleaning products).

GreenScreen® Summary Rating for Octamethylcyclotetrasiloxane [4]: Octamethylcyclotetrasiloxane was assigned a GreenScreen® Benchmark Score of 1 ("Avoid-Chemical of High Concern") as it has Very High persistence (P), Very High bioaccumulation (B), and Very High Ecotoxicity (chronic aquatic toxicity (CA)), which corresponds to GreenScreen® benchmark classifications 1a, 1b, 1c and 1d in CPA 2011, 2012a. As assessment of these endpoints revealed that octamethylcyclotetrasiloxane is a BM 1 chemical, assessment of additional endpoints was not performed. Additional authoritative A listings were sufficient to assign hazard scores for reproductive toxicity (R).

Figure 1: GreenScreen® Hazard Ratings for Octamethylcyclotetrasiloxane

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

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**[5]

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

Introduction
Octamethylcyclotetrasiloxane is commonly referred to as D4. It is a key ingredient in a variety of product formulations and a critical intermediate in the production of silicone polymers (ECHA 2014).

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.
[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

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

- PBT
  - Oregon DEQ-Priority Persistent Pollutants (OR P3): Priority Perisitent Pollutant-Tier 1
  - Environment Canada - Domestic Substances List (DSL): Persistent, Bioaccumulative and inherently Toxic (PBiT) to aquatic organisms
  - Environment Canada - Domestic Substances List (DSL): Persistent, Bioaccumulative and inherently Toxic (PBiT) to humans
  - Environment Canada - Domestic Substances List (DSL): DSL substances that are Persistent
  - Environment Canada - Domestic Substances List (DSL): DSL substances that are Bioaccumulative
- Reproductive
  - EC - Risk Phrases (EU R-Phrases): R62: Possible risk of impaired fertility
  - EC - CLP/GHS Hazard Statements (EU H-Statements): H361f Suspected of damaging fertility
  - New Zealand HSNO/GHS (GHS-New Zealand): 6.8B - Suspected human reproductive or developmental toxicants
  - EC - CLP Inventory (EU CMR (2)): Reproductive Toxicity - Category 2
- Endocrine
  - EC - Priority Endocrine Disrupters (EU ED): Category 1 - In vivo evidence of endocrine disruption activity
  - ChemSec - Substitute List (SIN): Equivalent concern, including endocrine disruption - Sin List 1.0 -
  - TEDX - Potential Endocrine Disruptors (TEDX): Potential Endocrine Disruptor
- Mammalian
  - New Zealand HSNO/GHS (GHS-New Zealand): 6.1D (dermal) - Acutely toxic
  - New Zealand HSNO/GHS (GHS-New Zealand): 6.1D (oral) - Acutely toxic
  - New Zealand HSNO/GHS (GHS-New Zealand): 6.1E (inhalation) - Acutely toxic
- Acute Aquatic
  - New Zealand HSNO/GHS (GHS-New Zealand): 9.1D (crustacean) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action
- Chronic Aquatic
  - EC - Risk Phrases (EU R-Phrases): R53: May cause long-term adverse effects in the aquatic environment.
  - EC - CLP/GHS Hazard Statements (EU H-Statements): H413 - Aquatic Chronic 4 - May cause long lasting harmful effects to aquatic life

- Flammable
    - New Zealand HSNO/GHS (GHS-New Zealand): 3.1C - Flammable Liquids: medium hazard
- Restricted List
    - German FEA - Substances Hazardous to Waters (VwVwS): Class 3 Severe Hazard to Waters -
    - Environment Canada - Toxic Substances List - Sched 1 (CEPA): CEPA Toxic
    - Environment Canada - Domestic Substances List (DSL): Inherently Toxic in the Environment -
    - Environment Canada - Domestic Substances List (DSL): Inherently Toxic to Humans: DSL substances that meet human health categorization criteria

PhysicoChemical Properties of Octamethylcyclotetrasiloxane

Octamethylcyclotetrasiloxane is a clear, odorless, oily liquid at room temperature that is insoluble in water. Its vapor pressure indicates that it is a highly volatile liquid and its log K_{ow} of 6.48 indicates that it is hydrophobic and has high potential for bioaccumulation.

Table 1: Physical and Chemical Properties of Octamethylcyclotetrasiloxane (CAS #556-67-2)

Property	Value	Reference
Molecular formula	$C_8H_{24}O_4Si_4$	ChemIDplus 2014
SMILES Notation	C[Si]1(O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)C	ChemIDplus 2014
Molecular weight	296.6176	ChemIDplus 2014
Physical state	Liquid	ECHA 2014
Appearance	Oily Liquid	HSDB 2006
Melting point	17.7ºC	ECHA 2014
Vapor pressure	132 Pa at 25ºC	ECHA 2014
Water solubility	0.056 mg/L at 23ºC	ECHA 2014
Dissociation constant	10.02 at 25ºC	ECHA 2014
Density/specific gravity	0.9558	HSDB 2006
Partition coefficient	Log K_{ow} = 6.49	ECHA 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 on any authoritative lists.
    - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
    - *Authoritative:* not on any authoritative lists.
    - *Screening:* not on any screening lists.

Reproductive Toxicity (R) Score (H, M, or L): M

Octamethylcyclotetrasiloxane was assigned a score of Moderate for reproductive toxicity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Moderate hazard for reproductive toxicity when the chemical is associated with the H-Statement H361f: Suspected of damaging fertility, R-Phrase R62: Possible risk of impaired fertility and Repr 2 in EU CMR(2) (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC - Risk Phrases (EU R-Phrases): R62: Possible risk of impaired fertility
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements): H361f Suspected of damaging fertility
  - *Authoritative:* EC - CLP Inventory (EU CMR (2)): Reproductive Toxicity - Category 2
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 6.8B - Suspected human reproductive or developmental toxicants
  - *Others:* US EPA - PPT Chemical Action Plans (EPA Action): Reproductive toxicity - TSCA Criteria met

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

- Authoritative and Screening Lists
  - *Authoritative:* EC - CLP Inventory (EU CMR (2)): Reproductive Toxicity - Category 2 (translates to a score of M for reproductive toxicity and/or developmental toxicity)
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* EC - Priority Endocrine Disrupters (EU ED): Category 1 - In vivo evidence of endocrine disruption activity
  - *Screening:* ChemSec - Substitute List (SIN): Equivalent concern, including endocrine disruption - Sin List 1.0
  - *Screening:* TEDX - Potential Endocrine Disruptors (TEDX): Potential Endocrine Disruptor
- High Throughput Screening (HTS) Data –
  - HTS data were identified for octamethylcyclotetrasiloxane using PubChem (http://pubchem.ncbi.nlm.nih.gov/).
  - The data included the following results:
    - Octamethylcyclotetrasiloxane was active in 0/7 androgen receptor agonist assays and 0/13 androgen receptor antagonist assays.
    - Octamethylcyclotetrasiloxane was active in 0/7 estrogen receptor-alpha agonist assays and 0/13 estrogen receptor-alpha antagonist assays.
    - Octamethylcyclotetrasiloxane was active in 0/3 thyroid receptor agonist assays and 0/7 thyroid receptor antagonist assays.
    - The activity of octamethylcyclotetrasiloxane towards the thyroid stimulating hormone receptor was not evaluated.

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 on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 6.1D (dermal) - Acutely toxic
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 6.1D (oral) - Acutely toxic
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 6.1E (inhalation) - Acutely toxic

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* not on any screening lists.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): Not Assessed

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 9.1D (crustacean) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action.

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

Octamethylcyclotetrasiloxane was assigned a score of Very High for chronic aquatic toxicity based on experimental chronic aquatic toxicity values. GreenScreen® criteria classify chemicals as a Very High hazard for chronic aquatic toxicity when chronic aquatic toxicity values are less than 0.1 mg/L (100 µg/L) (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC - Risk Phrases (EU R-Phrases): R53: May cause long-term adverse effects in the aquatic environment.
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements): H413 - Aquatic Chronic 4 - May cause long lasting harmful effects to aquatic life
  - *Screening:* not on any screening lists.
- ECHA 2014
    - NOEC ≥ 4.4 µg/L (*Oncorhynchus mykiss,* fish , 93-day)
    - NOEC = 7.9 µg/L (*Daphnia magna*, daphnia, 21-day)
    - No data were available for algae, but QSAR estimates indicate that algae should not be significantly more sensitive than fish and invertebrates.

Environmental Fate (Fate)

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

Octamethylcyclotetrasiloxane was assigned a score of Very High for persistence based on measured half-life in sediment, a conclusion by ECHA and association with the DSL screening list. GreenScreen® criteria classify chemicals as a Very High hazard for persistence when the half-life in sediment is greater than 180 days (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not on any authoritative lists.
  - *Screening:* Environment Canada - Domestic Substances List (DSL): DSL substances that are Persistent

- ECHA 2014
    - Octamethylcyclotetrasiloxane is not readily biodegradable but it does degrade in water by hydrolysis. The half-life for hydrolysis is dependent on the pH and temperature as described below
        - Hydrolysis half-life at pH 7 and 12°C (freshwater) = 16.7 days.
        - Hydrolysis half-life at pH 8 and 9°C (marine) = 2.9 days.
        - The main product from the hydrolysis reaction is known to be dimethylsilanediol, which itself is unlikely to possess PBT or vPvB properties.
    - Octamethylcyclotetrasiloxane is highly adsorptive to organic matter in suspended solids, sediment and soils, so the relevance of hydrolysis for such a hydrophobic substance is low. Octamethylcyclotetrasiloxane has a very long degradation half-life in sediment, of the order of 242 days at 24°C under aerobic conditions and 365 days at 24°C under anaerobic conditions. The half-life at lower temperatures (e.g. 12°C) would be expected to be longer than these values.
- U.S. EPA 2012
    - Biowin predicted that octamethylcyclotetrasiloxane is not readily biodegradable. Fugacity modeling indicates that 47.9% will partition to soil with a half-life of 75 days, 22.3% will partition to water with a half-life of 37.5 days, and 15.1% will partition to air with a half-life of 10.6 days. See Appendix D for model output.
- Based on the above data, ECHA 2014 concluded that octamethylcyclotetrasiloxane can be considered to meet the REACH criteria for a persistent (P) and very persistent (vP) substance based on the measured and predicted half-lives in sediment.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vH
Octamethylcyclotetrasiloxane was assigned a score of Very High for bioaccumulation based on an experimental BCF of 13400. GreenScreen® criteria classify chemicals as a Very High hazard for bioaccumulation when the BCF is greater than 5000 (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* not on any authoritative lists.
    - *Screening:* DSL: DSL substances that are Bioaccumulative
- ECHA 2014
    - In a GLP-compliant study conducted according to EPA OTS 797.1520 (Fish Bioconcentration Test-Rainbow Trout) protocol, a steady-state BCF value of 12400 and kinetic BCF value of 13400 were determined for octamethylcyclotetrasiloxane.
    - It was concluded in ECHA 2014 PBT assessment report for octamethylcyclotetrasiloxane that it meets the REACH criteria for B and vB based on the fish BCF and overall weight of evidence.

Physical Hazards (Physical)

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

- Authoritative and Screening Lists
    - *Authoritative:* not on any authoritative lists.
    - *Screening:* not on any screening lists.

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

- Authoritative and Screening Lists
    - *Authoritative:* not on any authoritative lists.

- *Screening:* New Zealand HSNO/GHS (GHS-New Zealand): 3.1C - Flammable Liquids: 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 Octamethylcyclotetrasiloxane (CAS #556-67-2)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	**Octamethylcyclotetrasiloxane**	**556-67-2**	DG	**M**	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	**vH**	**vH**	**vH**	DG	DG

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Octamethylcyclotetrasiloxane	1

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

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
Octamethylcyclotetrasiloxane	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 Octamethylcyclotetrasiloxane (CAS #556-67-2)

Octamethylcyclotetrasiloxane (D4)

CAS RN: 556-67-2

Synonyms: Cyclotetrasiloxane, octamethyl-; CYCLIC DIMETHYLSILOXANE TETRAMER

Detailed Direct Hazard Listings — Quickscreen

PBT	**Oregon DEQ - Priority Persistent Pollutants (OR P3)** Priority Persistent Pollutant - Tier 1 - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
PBT	**Environment Canada - Domestic Substances List (DSL)** Persistent, Bioaccumulative and inherently Toxic (PBiT) to aquatic organisms - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
PBT	**Environment Canada - Domestic Substances List (DSL)** Persistent, Bioaccumulative and inherently Toxic (PBiT) to humans - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
REPRODUCTIVE	**US EPA - PPT Chemical Action Plans (EPA Action)** Reproductive toxicity - TSCA Criteria met
PBT	**EC - ESIS-PBT System (EU PBT)** Under PBT evaluation - Not included in GreenScreen - HPD
REPRODUCTIVE	**EC - Risk Phrases (EU R-Phrases)** R62: Possible risk of impaired fertility. - GreenScreen Benchmark Unspecified (LT-U) - HPD
REPRODUCTIVE	**EC - CLP/GHS Hazard Statements (EU H-Statements)** H361f Suspected of damaging fertility - GreenScreen Benchmark Unspecified (LT-U) - HPD
REPRODUCTIVE	**New Zealand HSNO/GHS (GHS-New Zealand)** 6.8B - Suspected human reproductive or developmental toxicants - GreenScreen Benchmark Unspecified (LT-U)
REPRODUCTIVE	**EC - CLP Inventory (EU CMR (2))** Reproductive Toxicity - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
ENDOCRINE	**EC - Priority Endocrine Disrupters (EU ED)** Category 1 - In vivo evidence of endocrine disruption activity - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
ENDOCRINE	**ChemSec - Substitute List (SIN)** Equivalent concern, including endocrine disruption - Sin List 1.0 - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
ENDOCRINE	**TEDX - Potential Endocrine Disruptors (TEDX)** Potential Endocrine Disruptor - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
MAMMALIAN	**New Zealand HSNO/GHS (GHS-New Zealand)** 6.1D (dermal) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	**New Zealand HSNO/GHS (GHS-New Zealand)** 6.1D (oral) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)

ACUTE AQUATIC	**New Zealand HSNO/GHS (GHS-New Zealand)** 9.1D (crustacean) - Slightly harmful in the aquatic environment or are otherwise designed for biocidal action - GreenScreen Benchmark Unspecified (LT-U)
CHRON AQUATIC	**EC - Risk Phrases (EU R-Phrases)** R53: May cause long-term adverse effects in the aquatic environment. - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only
CHRON AQUATIC	**EC - CLP/GHS Hazard Statements (EU H-Statements)** H413 - Aquatic Chronic 4 - May cause long lasting harmful effects to aquatic life - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only
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 Persistent - GreenScreen Benchmark Unspecified (LT-U)
PBT	**US EPA - PPT Chemical Action Plans (EPA Action)** High bioaccumulation potential - TSCA Criteria met
PBT	**US EPA - PPT Chemical Action Plans (EPA Action)** Medium environmental persistence - TSCA Criteria met
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 (inhalation) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	**German FEA - Substances Hazardous to Waters (VwVwS)** Class 3 Severe Hazard to Waters - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
RESTRICTED LIST	**US EPA - PPT Chemical Action Plans (EPA Action)** TSCA Work Plan chemical - Action Plan in development - Not included in GreenScreen - HPD
RESTRICTED LIST	**US EPA - PPT Chemical Action Plans (EPA Action)** TSCA Work Plan chemical - planned for assessment - Not included in GreenScreen - HPD
RESTRICTED LIST	**Hazardous 100 (SCHF)** Chemicals of high concern - Not included in GreenScreen
RESTRICTED LIST	**Environment Canada - Toxic Substances List - Sched 1 (CEPA)** CEPA Toxic - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	**Environment Canada - Domestic Substances List (DSL)** Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	**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)

Compound Group Hazard Listings

RESTRICTED LIST	**US EPA - PPT Chemical Action Plans (EPA Action)** TSCA Work Plan chemical - Action Plan in development - Not included in GreenScreen - HPD
RESTRICTED LIST	**CA SCP Candidate Chemicals** Full Candidate Chemical List - Not included in GreenScreen
RESTRICTED LIST	**Living Future - Living Building Red List (ILFI Red)** Red List substance to avoid in Living Building Challenge V3 projects - Not included in GreenScreen
EXEMPT	**US EPA - Exempt VOCs** Non smog forming exempt VOCs - Not included in GreenScreen

APPENDIX D: EPISuite Output for Octamethylcyclotetrasiloxane (CAS #556-67-2)

CAS Number: 556-67-2
SMILES: C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM: Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT: 296.62
---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log K_{ow} (octanol-water): ------
Boiling Point (deg C): ------
Melting Point (deg C): ------
Vapor Pressure (mm Hg): ------
Water Solubility (mg/L): ------
Henry LC (atm-m^3/mole): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (K_{ow}WIN v1.68 estimate) = 6.79
Log K_{ow} (Exper. database match) = 6.74
Exper. Ref: SEHSC (2009); average

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 159.41 (Adapted Stein & Brown method)
Melting Pt (deg C): 1.78 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 1.18 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C): 158 (Mean VP of Antoine & Grain methods)
MP (exp database): 17.5 deg C
BP (exp database): 175.8 deg C
VP (exp database): 1.05E+00 mm Hg (1.40E+002 Pa) at 25 deg C

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 0.06124
log K_{ow} used: 6.74 (expk_{ow} database)
no-melting pt equation used
Water Sol (Exper. database match) = 0.005 mg/L (25 deg C)
Exper. Ref: DOW CORNING (1987)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.17229 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 8.72E-002 atm-m^3/mole (8.84E+003 Pa-m^3/mole)
Group Method: Incomplete
Exper Database: 1.17E-01 atm-m^3/mole (1.19E+004 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: 7.520E+000 atm-m^3/mole (7.620E+005 Pa-m^3/mole)
VP: 1.18 mm Hg (source: MPBPVP)
WS: 0.0612 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 6.74 (exp database)
Log K_{aw} used: 0.680 (exp database)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 6.060
Log K_{oa} (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.6063
Biowin2 (Non-Linear Model): 0.2309
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.5437 (weeks-months)
Biowin4 (Primary Survey Model): 3.4198 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): -0.1670
Biowin6 (MITI Non-Linear Model): 0.0028
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.1995
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 140 Pa (1.05 mm Hg)
Log K_{oa} (K_{oa}win est): 6.060
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model: 2.14E-008
Octanol/air (K_{oa}) model: 2.82E-007
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 7.74E-007
Mackay model: 1.71E-006
Octanol/air (K_{oa}) model: 2.25E-005

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 1.1968 E-12 cm^3/molecule-sec
Half-Life = 8.937 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 107.246 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
1.24E-006 (Junge-Pankow, Mackay avg)

2.25E-005 (K_{oa} method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
K_{oc}: 1.444E+004 L/kg (MCI method)
Log K_{oc}: 4.159 (MCI method)
K_{oc}: 7.067E+005 L/kg (K_{ow} method)
Log K_{oc}: 5.849 (K_{ow} method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 4.114 (BCF = 1.3e+004 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 1.7346 days (HL = 54.28 days)
Log BCF Arnot-Gobas method (upper trophic) = 3.882 (BCF = 7620)
Log BAF Arnot-Gobas method (upper trophic) = 6.249 (BAF = 1.774e+006)
log K_{ow} used: 6.74 (expk_{ow} database)

Volatilization from Water:
Henry LC: 0.117 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 1.766 hours
Half-Life from Model Lake: 163.7 hours (6.82 days)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 95.47 percent
Total biodegradation: 0.61 percent
Total sludge adsorption: 83.53 percent
Total to Air: 11.33 percent
(using 10000 hr. Bio P,A,S)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 99.07 percent
Total biodegradation: 35.37 percent
Total sludge adsorption: 61.35 percent
Total to Air: 2.35 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	15.1	254	1000
Water	22.3	900	1000
Soil	47.9	1.8e+003	1000
Sediment	14.7	8.1e+003	0

Persistence Time: 397 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/

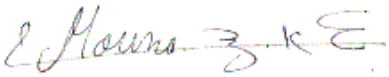
International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

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

Octamethylcyclotetrasiloxane GreenScreen® Evaluation Prepared by:



Mouna Zachary, Ph.D.
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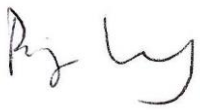
ToxServices LLC

Octamethylcyclotetrasiloxane GreenScreen® Evaluation QC'd by:



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