Propylene Glycol (CAS# 57-55-6) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

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GreenScreen® Executive Summary for Propylene Glycol (CAS #57-55-6)

Propylene glycol is a chemical that functions as a solvent, extractant, preservative, plasticizer, skin-conditioning agent, viscosity-decreasing agent, humectant, and in polymer production.

Propylene glycol was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Moderate Group I Human Toxicity (reproductive toxicity (R) and developmental toxicity (D)). This corresponds to GreenScreen® benchmark classification 2e in CPA 2011. Data gaps (DG) exist for endocrine activity (E), neurotoxicity repeated dose (Nr*) and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), propylene glycol meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if propylene glycol were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

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 2 ("Use but Search for Safer Substitutes") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for Propylene Glycol

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*											
L	**L**	**M**	*M*	DG	**L**	DG	*M*	**M**	DG	**L**	DG	**L**	**L**	**L**	**L**	**vL**	**vL**	*L*	**L**

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.

GreenScreen® Assessment for Propylene Glycol (CAS #57-55-6)

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

Chemical Name: Propylene glycol

CAS Number: 57-55-6

GreenScreen® Assessment Prepared By:
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Organization: ToxServices LLC
Date: February 20, 2012 (Original)
October 14, 2014 (Update)
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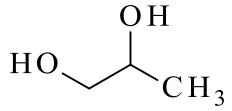
Organization: ToxServices LLC
Date: February 20, 2014 (Original)
December 1, 2014 (Update)

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

Chemical Structure(s):



(ChemIDplus 2014)

Also called: 1,2-Propanediol, 2,3-Propanediol, 2-Hydroxypropanol, Methylethylene glycol (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
As propylene glycol has a relatively complete dataset, no surrogate was sought.

Identify Applications/Functional Uses: (HSDB 2010)
1. Solvent
2. Extractant
3. Preservative
4. Plasticizer in aqueous film-coating formulations
5. Skin-conditioning agent, viscosity-decreasing agent and humectant in cosmetics
6. Polymer production

[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

GreenScreen® Summary Rating for Propylene Glycol[4]: Propylene glycol was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Moderate Group I Human Toxicity (reproductive toxicity (R) and developmental toxicity (D)). This corresponds to GreenScreen® benchmark classification 2e in CPA 2011, 2012a. Data gaps (DG) exist for endocrine activity (E), neurotoxicity repeated dose (Nr*) and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), propylene glycol meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if propylene glycol were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Ratings for Propylene Glycol

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*										
L	L	M	*M*	DG	L	DG	*M*	M	DG	L	DG	L	L	L	L	vL	vL	*L*	L

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]

As propylene glycol is readily biodegradable (see persistence section below), no feasible and relevant environmental transformation products are expected to be formed.

Introduction

Propylene glycol has numerous functions in industrial processes and consumer products. It is manufactured from hydroxyacetone by yeast reduction, by non-catalytic liquid-phase hydration of propylene oxide at 100 – 200ºC (major industrial method), by chlorination and treatment with sodium carbonate from propylene, and by heating glycerol with sodium hydroxide (HSDB 2010).

ToxServices assessed propylene glycol 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

[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.

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 propylene glycol can be found in Appendix C and a summary of the results can be found below:

Restricted list
German FEA VwVwS – Class 1 low hazard to waters
Environmental Canada – DSL inherently toxic to humans
Developmental
NTP-OHAaT – G: clear evidence of no adverse developmental toxicant effects
NTP-OHAaT – G: clear evidence of no adverse reproductive toxicant effects

PhysicoChemical Properties of Propylene Glycol

Propylene glycol is a colorless viscous liquid at ambient temperature. Its vapor pressure indicates that it can form a vapor. Propylene glycol is miscible in water and the low partition coefficient of -0.92 indicates that it is hydrophilic with low potential to bioaccumulate in the aquatic biota.

Table 1: Physical and Chemical Properties of Propylene Glycol (CAS #57-55-6)

Property	Value	Reference
Molecular formula	C3-H8-O2	ChemIDPlus 2014
SMILES Notation	C([C@@H](C)O)O	ChemIDPlus 2014
Molecular weight	76.0942	ChemIDPlus 2014
Physical state	Liquid	HSDB 2010
Appearance	Colorless viscous liquid	HSDB 2010
Melting point	-60ºC	HSDB 2010
Vapor pressure	0.08 mmHg	UNEP 2001
Water solubility	10^6 mg/L at 20ºC (miscible)	HSDB 2010
Dissociation constant	pKa = 14.8 at 25ºC	HSDB 2010
Density/specific gravity	1.0361 g/cm^3 at 20ºC	HSDB 2010
Partition coefficient	-0.92	HSDB 2010

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

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

Propylene glycol was assigned a score of Low for carcinogenicity based on negative data. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate data are available and negative, there are no structural alerts, and they are not classifiable under GHS (CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists

- UNEP 2001
    - *Oral:* A non-GLP compliant 2 year chronic toxicity/carcinogenicity study (method not reported) was conducted using male and female CD rats (number not reported). Rats were administered doses of up to 2,100 mg/kg of the propylene glycol (purity not reported) daily for 2 years. No evidence of any treatment related tumors were reported under the test conditions. Limited details were available for this study.
    - *Oral:* A non-GLP compliant 2 year chronic toxicity/carcinogenicity study (method not reported) was conducted using male and female Beagle dogs (number not reported). Dogs were administered doses of up to 5,000 mg/kg of propylene glycol daily for 2 years. Tumor incidences were unchanged in male and female dogs when compared to the controls. No further details were provided for this study.
    - *Dermal:* In a skin painting study, propylene glycol was administered to female mice at 2, 10 or 21 mg/day over the life time. No increase in dermal tumors was observed.
    - *Dermal:* When used as a vehicle (dose not specified) in an ear painting study in rats, propylene glycol did not induce tumors after 10 – 14 months treatment.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L

Propylene glycol was assigned a score of Low for mutagenicity/genotoxicity based on experimental data *in vitro* and *in vivo*. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when adequate data are available and negative for both mutagenicity and clastogenicity, there are no structural alerts, and they are not classifiable under GHS (CPA 2012a).

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- UNEP 2001
    - A (GLP status not reported) bacterial reverse mutation assay (method not reported) was conducted utilizing *Salmonella typhimurium* tester strains TA92, TA94, TA98, TA100, TA1535 and 1537 in the presence of metabolic activation at concentrations up to 10 mg/plate. No increase in revertants was observed and propylene glycol was reported as negative for mutagenicity under the tested conditions.
    - A (GLP status not reported) bacterial reverse mutation assay (method not reported) was conducted utilizing *Salmonella typhimurium* tester strains TA98, TA100, TA1535 and TA1537 at concentrations of up to 300 µmol/plate in the absence of metabolic activation. No increase in revertants was observed and propylene glycol was reported as negative for mutagenicity under the tested conditions.
    - A GLP compliant chromosomal aberration test (OECD 473) was conducted utilizing cultured human lymphocytes at concentrations of up to 3,810 µg/ml with and without metabolic activation. Propylene glycol showed no evidence of clastogenic effects under all tested conditions and was reported as negative for genotoxicity.
    - A (GLP status not reported) chromosomal aberration test (method not reported) was conducted utilizing Chinese Hamster Lung (CHL) fibroblasts at concentrations of up to 32 mg/ml in the absence of metabolic activation. Cells at 32 mg/ml (420 mM) showed a 38% increase in structural aberrations. However, at 32 mg/ml significant cytotoxicity was reported, and this concentration is above the 10 mM maximum concentration recommended by modern guidelines. Therefore, the results of this study are inconclusive as cytotoxic and osmotic destabilizing effects could cause the study results to be unreliable. In addition, the lower two doses tested showed no signs of cytogenic activity.
    - A non-GLP compliant cytogenetic assay (method not reported) was conducted using male Sprague-Dawley rats (15/group). Rats were administered a single dose or five consecutive

daily doses of 0, 30, 2,500, or 5,000 mg/kg and then sacrificed at 6, 24, or 48 hours following treatment. Increases in chromosomal aberrations were reported in the mid and high-dose group. However, these effects were well within historic ranges and it was concluded that ethylene glycol was not genotoxic.

- A (GLP status not reported) micronucleus assay (method not reported) was conducted in male mice at intraperitoneal doses of 0, 2,500, 5,000, 10,000 and 15,000 mg/kg (single exposure). Propylene glycol did not induce formation of micronuclei in the bone marrow 18 hours after exposure.
- In two rat dominant lethal assays, single gavage dose or five daily gavage doses of 30, 2,500 and 5,000 mg/kg did not produce positive results. The occasional statistically-increased finding in mid and high does animals were within historic range, and the statistical significance was attributed to unrepresentative control data.

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

Propylene glycol was assigned a score of Moderate for reproductive toxicity based on experimental data indicating reduced fertility and ovary weights in rats after inhalation exposure. GreenScreen® criteria classify chemicals as a Moderate hazard for reproductive toxicity when there is limited or marginal evidence of reproductive toxicity in animals (CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists
- UNEP 2001
  - *Oral:* A (GLP status not reported) two generation toxicity study (method not reported) was conducted using male and female CD-1 mice (20/sex/group). Mice were administered doses of 0, 1,800, 4,800, and 10,100 mg/kg from 7 days before mating to 98 days following mating in drinking water. Slight increases in water consumption were observed in all parental dose groups. Body weights were unaffected. Necropsy of F1 adults revealed no effects on mating, fertility or the number, weight or viability of F2 pups. The study authors reported a NOAEL of 10,100 mg/kg based on no effects at the top dose.
- ATSDR 2008
  - *Inhalation:* A (GLP status not reported) two-generation toxicity study (method not reported) was conducted in Sprague-Dawley rats. Animals were exposed via inhalation to propylene glycol at 0, 300, 1,000 or 3,000 ppm for 6 hours/day for 5 weeks before mating, and 6 hours/day and 7 days/week during mating and gestation. Decreased fertility and ovary weights were found in maternal rats, and decreased body weight, reduced survival and litter size, slight delays in puberty onset and histological changes in the liver and thymus were reported in F1 and F2 offspring of the affected dams. No further details were provided.

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

Propylene glycol was assigned a score of Moderate for developmental toxicity based on experimental data. GreenScreen® criteria classify chemicals as a Moderate hazard for developmental toxicity when there is limited or marginal evidence of developmental toxicity in animals (CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists
- UNEP 2001
  - *Oral:* A non-GLP compliant developmental toxicity study (method not reported) was conducted using female Wistar rats (25/dose). Rats were administered does of 0, 16, 74.3, 345, and 1,600 mg/kg on days 6 to 15 of gestation via oral gavage. No effects were reported on live litters, total or average number of implant sites, total and partial resorptions, the total

and average number of five fetuses and their sex ratio, and the number of dead fetuses or fetal weight. Based on the available data, a NOAEL of 1,600 mg/kg was reported by the study authors.

- *Oral:* A non-GLP compliant developmental toxicity study (method not reported) was conducted using female Dutch-belted rabbits (n=15 to 20). Rabbits were administered doses of 0, 12.3, 57.1, 267, and 1,230 mg/kg of the test substance on days 6 to 18 of gestation via oral gavage. No effects were reported on live litters, total or average number of implant sites, total and partial resorptions, the total and average number of five fetuses and their sex ratio, and the number of dead fetuses or fetal weight. Based on the available data, a NOAEL of 1,230 mg/kg was reported by the study authors.
- *Oral:* A non-GLP compliant developmental toxicity study (method not reported) was conducted using female CD-1 mice (n=25 to 28). Mice were administered doses of 0, 16, 74.3, 345, and 1,600 mg/kg of the test substance on days 6 to 15 of gestation via oral gavage. No effects were reported on live litters, total or average number of implant sites, total and partial resorptions, the total and average number of five fetuses and their sex ratio, and the number of dead fetuses or fetal weight. Based on the available data, a NOAEL of 1,600 mg/kg was reported by the study authors.
- *Oral:* A non-GLP compliant developmental toxicity study (method not reported) was conducted using female (strain not reported) hamsters (n=24 to 27). Hamsters were administered doses of 0, 15.5, 72.0, 334.5, and 1,550 mg/kg of the test substance on days 6 to 10 of gestation via oral gavage. No effects were reported on live litters, total or average number of implant sites, total and partial resorptions, the total and average number of five fetuses and their sex ratio, and the number of dead fetuses or fetal weight. Based on the available data, a NOAEL of 1,550 mg/kg was reported by the study authors.

- ATSDR 2008
  - *Inhalation:* In the previously described two-generation toxicity study (method not reported) in Sprague-Dawley rats, animals were exposed via inhalation to propylene glycol at 0, 300, 1,000 or 3,000 ppm for 6 hours/day for 5 weeks before mating, and 6 hours/day and 7 days/week during mating and gestation. Decreased fertility and ovary weights were found in maternal rats, and decreased body weight, reduced survival and litter size, slight delays in puberty onset and histological changes in the liver and thymus were reported in F1 and F2 offspring of the affected dams. No further details were provided.
  - *Inhalation:* A developmental toxicity study was conducted in New Zealand White rabbits and Fischer-344 rats. Animals were exposed to propylene glycol at 0, 50, 150 or 300 ppm for 6 hours/day on gestational days 7 – 19 (rabbits) or 6 – 15 (rats). No embryo-fetotoxicity, or teratogenicity was observed.
  - *Inhalation:* Chicken embryos (50 in total) were exposed to propylene glycol through the air sac at 0.02 µg/egg. Ultra structural changes were found in the bursa of Fabricius, which is a blind saclike structure that opens the hindgut, bladder and genital ducts and that serves as a primary lymphoid organ for the normal development of immunological function. No further details were reported.
- The weight of evidence indicates that propylene glycol is not a developmental toxicant by the oral route. A 2-generation inhalation toxicity study reported developmental toxicity in the form of decreased body weight, reduced survival and litter size, slight delays in puberty onset and histological changes in the liver and thymus in F1 and F2 offspring in the presence of maternal reproductive toxicity (systemic toxicity status not reported). An inhalation developmental toxicity at lower concentrations did not report any developmental toxicity. While the developmental effects observed in the 2-generation study may be related to maternal toxicity, the lack of sufficient data

made it impossible to discern if these effects are secondary or specific. Therefore, ToxServices conservatively assigned a score of Moderate with low confidence.

Endocrine Activity (E) Score (H, M, or L): DG
Propylene glycol was assigned a score of Data Gap for endocrine disruption based on lack of data.

- Authoritative and Screening Lists
  - Not on any authoritative or 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 propylene glycol using PubChem (http://pubchem.ncbi.nlm.nih.gov/).
  - The data included the following results:
    - Propylene glycol was active in 0/2 androgen receptor agonist assays and 0/13 androgen receptor antagonist assays.
    - Propylene glycol was active in 0/26 estrogen receptor-alpha agonist assays and 0/1 estrogen receptor-alpha antagonist assays.
    - Propylene glycol was active in 0/6 thyroid receptor agonist assays and 0/14 thyroid receptor antagonist assays.
    - Propylene glycol was active in 0/5 thyroid stimulating hormone receptor agonist assays and 0/1 thyroid stimulating hormone receptor antagonist assay.
- These data are insufficient to assign a score for endocrine activity.

Group II and II* Human Health Effects (Group II and II* Human)
Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): L
Propylene glycol was assigned a score of Low for acute toxicity based on oral, dermal and inhalation LD/C_{50} values. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral and dermal LD_{50} values > 2,000 mg/kg and inhalation LC_{50} > 5 mg/L (dust/mist) (CPA 2012a).

- Authoritative and Screening Lists
  - Not listed on authoritative or screening lists
- UNEP 2001 -
  - An Oral LD_{50} value of 22,000 mg/kg in (strain not reported) rats.
  - An Oral LD_{50} value of 24,900 mg/kg in (strain not reported) mice.
  - An Oral LD_{50} value of 19,700 mg/kg in (strain not reported) guinea pigs.
  - A Dermal LD_{50} value of 20,800 mg/kg in (strain not reported) rabbits.
- ECHA 2014
  - A 2-h inhalation LC_{50} value of > 31.7 mg/L for propylene glycol aerosols in (strain not reported) rabbits

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)* (vH, H, M, or L):** DG
Propylene glycol was assigned a score of Data Gap for systemic toxicity (single dose) based on lack of data.

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- No data were identified.

***Group II* Score (repeated dose)* (H, M, or L):** *M*
Propylene glycol was assigned a score of Moderate for systemic toxicity (repeated dose) based on inhalation LOAEC of 0.11 mg/L/day. GreenScreen® criteria classify chemicals as a Moderate hazard for systemic toxicity (repeated dose) when inhalation LOAECs are between 0.02 and 0.2 mg/L/day (dust/mist) (CPA 2012a). Confidence level was reduced due to lack of data regarding whether adverse effects would occur at 0.02 mg/L/day.

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- UNEP 2001
    - *Oral:* A non-GLP compliant 2 year chronic toxicity/carcinogenicity study (method not reported) was conducted using male and female CD rats (number not reported). Rats were administered doses of up to 2,100 mg/kg of the propylene glycol (purity not reported) daily for 2 years. No systemic effects were reported under the test conditions. Limited details were available for this study. ToxServices identified the NOAEL at 2,100 mg/kg/day.
    - *Oral:* A non-GLP compliant 2 year chronic toxicity/carcinogenicity study (method not reported) was conducted using male and female Beagle dogs (number not reported). Dogs were administered doses of up to 5,000 mg/kg of propylene glycol daily for 2 years. Minor red blood cell changes (significance not reported) were the only reported effect. No further details were provided for this study. ToxServices identified the NOAEL at 5,000 mg/kg/day.
    - *Oral:* Several other repeat dose studies were identified with limited details available. No significant effects were reported except for species specific formation of Heinz bodies in cats administered 443 mg/kg of propylene glycol.
- ECHA 2014
    - *Inhalation:* A (GLP status not reported) subchronic inhalation toxicity study was conducted in Sprague-Dawley rats. Animals (19/sex/dose) were exposed nose-only to propylene glycol aerosols (mass median aerodynamic diameter: < 2.22 and < 1.96 μm for mid and high dose groups)) at 0, 0.16, 1.01 or 2.18 mg/L for 6 hours/day, 5 days/week for 90 days. Parameters examined include clinical signs, body weights, food consumption, hematology, clinical chemistry and gross and histopathological examinations. Treatment-related nasal hemorrhage was found in all exposed groups. There was a dose-dependent reduction in body weight (up to 7%) in females and males (up to 6%), but the effect was only statistically significant at the high dose in females. These were correlated with a significant reduction in feed consumption in all treated females and high dose males. A statistically significant decrease in mean corpuscular hemoglobin concentration was found in high dose females and significant decrease in white blood cell count, banded neutrophil count and lymphocyte count were reported in mid and high dose females. Statistically significant decreases in serum gamma-glutamyl transferase and changes (unspecified) in serum protein, albumin and cholesterol were found in high dose males. An inverse dose-dependent relationship was found for serum aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase,

gamma-glutamyl transferase, serum protein, albumin, cholesterol and inorganic phosphate in males (statistical significance not reported). Absolute organ weight changes were reported for the lung, spleen liver and kidney. Relative organ weight changes include significantly decreased spleen weights in high dose males and increased lung weights in low dose males. Thickening of the respiratory epithelium at the mid and high doses was the only microscopic finding. The ECHA dossier identified a NOAEC of 1.01 mg/L for females based on decreased body weights at the LOAEC of 2.18 mg/L, and a NOAEC of 2.18 mg/L for males. The nasal hemorrhaging effect was not considered an adverse effect, with the LOEC of 0.16 mg/L. ToxServices conservatively used the LOEC of 0.16 mg/L this assessment, which is equivalent to 0.11 mg/L/day after adjustment for a 7 day/week exposure frequency[6].

Neurotoxicity (N)

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

Propylene glycol was assigned a score of Moderate for neurotoxicity (single dose) based on transient narcosis and CNS depression in humans and animals. GreenScreen® criteria classify chemicals as a Moderate hazard for neurotoxicity (single dose) when classified to GHS category 3 based on transient narcotic effects (CPA 2012a).

- Authoritative and Screening Lists
  - Not present on any authoritative or screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- ATSDR 2008
  - In humans, the primary clinical signs of acute toxicity to propylene glycol are consequences of CNS effects such as depression and lactic acid acidosis from extremely high doses. In animals, symptoms of acute oral exposure to propylene glycol include CNS depression or narcosis.

***Group II* Score (repeated dose)* (H, M, or L):** DG

Propylene glycol was assigned a score of Data Gap for neurotoxicity (repeated dose) based on lack of data.

- Authoritative and Screening Lists
  - Not present on any authoritative or screening lists.
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- No data were identified.

Skin Sensitization (SnS) Group II* Score (H, M, or L): L

Propylene glycol was assigned a score of Low for skin sensitization based on measured data. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and negative, there are no structural alerts, and they are not classifiable under GHS (CPA 2012a).

- Authoritative and Screening Lists
  - Not on authoritative or screening lists.
- UNEP 2001
  - A GLP compliant repeat insult patch test (method not reported) was conducted using human volunteers (n=104). Approximately 0.2 ml of a 50% aqueous dilution of propylene glycol was applied under semi-occlusive dressing to humans for 24 hours, 3 days a week, for 3 weeks. A challenge dose was applied 2 weeks after the final treatment. No effects were

[6] 0.16 mg/L x 5 days/7 days = 0.11 mg/L/day.

reported following the challenge dose and propylene glycol was reported as negative for skin sensitization.
    - A second non-GLP compliant patch test (method not reported) was conducted using human volunteers (n=204). Ten consecutive induction applications of 0.5g in a 12% dilution were applied to the lateral portion of the arm under occlusive conditions. A challenge dose (conditions not specified) was applied following a two week rest period and no reactions were observed. Propylene glycol was reported as negative for skin sensitization by the study authors.
- ECHA 2014 (only studies marked as key studies were described below)
    - A guinea pig maximization test (equivalent or similar to OECD guideline 406) was conducted (GLP status not reported) with female Dunkin-Hartley guinea pigs. Animals were induced dermally with the neat substance twice and challenged on day 21 with the neat substance. No positive reactions were observed in all 20 animals.
    - A mouse local lymph node assay (equivalent or similar to OECD guideline 429) was conducted (GLP status not reported) in CBA mice at propylene glycol concentrations of 50 and 100%. Stimulation indices were 1.2 and 1.6 for the two concentrations, respectively, which are below the cut-off of 3 for positive reactions. Therefore, propylene glycol is not considered a dermal sensitizer.
    - A split adjuvant test (according to standard procedure of Maguire, 1973) was conducted (GLP status not reported) in female Dunkin-Hartley guinea pigs. Propylene glycol at 100% did not induce any positive reactions in any of the 30 animals.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG
Propylene glycol was assigned a score of Data Gap for respiratory sensitization based on lack of data.
- Authoritative and Screening Lists
    - Not on any authoritative or screening list
- No data were identified.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): L
Propylene glycol was assigned a score of Low for skin irritation/corrosivity based on measured data. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and negative, there are no structural alerts, and they are not classifiable under GHS (CPA 2012a).
- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- UNEP 2001
    - An (GLP status not reported) acute dermal irritation/corrosion study (OECD 404) was conducted using female New Zealand rabbits (n=6). Rabbits were exposed to 0.5 ml of propylene glycol (purity not reported) for an unreported amount of time. Animals were examined at 1, 24, 48, and 72 hours following patch removal. An average score of 0.1 was reported for erythema. Propylene glycol was reported as not irritating to the skin of rabbits by the study authors. An average score of greater than 1.5 at 24, 48, and 72 hours is required for classification as a GHS skin irritant.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): L
Propylene glycol was assigned a score of Low for eye irritation/corrosivity based on negative data. GreenScreen® criteria classify chemicals as a Low hazard for eye irritation/corrosivity when adequate

data are available and negative, there are no structural alerts, and they are not classifiable under GHS (CPA 2012a).

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- UNEP 2001
    - A (GLP status not reported) acute eye irritation/corrosion study (OECD 405) was conducted using New Zealand white rabbits (sex not reported, n=6). 0.1 ml of an undiluted propylene glycol was instilled into the eyes of rabbits for an unreported amount of time. Rabbits were examined at 4, 24, 48, 72, and 96 hours. There were no signs of chemosis, corneal opacity, or surface corneal damage at all doses. Propylene glycol was reported as non-irritating to the eyes of rabbits by the study authors.

Ecotoxicity (Ecotox)

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

Propylene glycol was assigned a score of Low for acute aquatic toxicity based on measured data. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute aquatic L/EC_{50} values > 100 mg/L (CPA 2012a).

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists.
- UNEP 2001
    - An LC_{50} value of 51,600 mg/L was identified in *Oncorhynchus mykiss* (fish, 96-hr) (OECD 203).
    - An LC_{50} value of 46,500 to 51,400 mg/L was identified in *Pimephalas promelas* (fish, 96-hr) (OECD 203).
    - An LC_{50} value of 43,500 mg/L was identified in *Daphnia magna* (invertebrate, 48-hr) (OECD 202).
    - An LC_{50} value of 18,800 mg/L was identified in *Mysidopsis bahia* (invertebrate, 96-hr).
    - An LC_{50} value of 18,340 mg/L was identified in *Ceriodaphnia sp.* (invertebrate, 48-hr).
    - An EC_{50} value of 19,000 mg/L was identified in *Selenastrum capricornutum* (algae, 96-hr) (OECD 201).
    - An EC_{50} value of 19,100 mg/L was identified in *Skeletonema costatum* (algae, 96-hr) (OECD 201).

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

Propylene glycol was assigned a score of Low for chronic aquatic toxicity based on measured data. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when ChV > 10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists.
- UNEP 2001
    - 14-Day NOEC = 15,000 mg/L for *Selenastrum capricornutum* (green algae, OECD 201)
    - 14-Day NOEC ≤ 5,300 mg/L in *Skeletonema costatum* (green algae, OECD 201)
    - 7-day NOEC (reproduction) = 13,020 mg/L in *Ceriodaphnia dubia* (aquatic invertebrate)
    - 7-day NOEC < 11, 530 mg/L for growth in fathead minnow

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): vL
Propylene glycol was assigned a score of Very Low for persistence based on measured data. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence when meeting the 10-day window in ready biodegradability tests and the major partitioning compartment is water/soil/sediment (CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists
- UNEP 2001
  - A non-GLP compliant biodegradation study (method not reported) was conducted under aerobic conditions in activated domestic sludge. Propylene glycol was reported as 68% biodegradable after 10 days and 79% biodegradable after 20 days, and was reported as readily biodegradable under the tested conditions.
  - A (GLP status not reported) biodegradation study (method not reported) was conducted under aerobic conditions using soil microcosm. Propylene glycol was reported as 100% degradable after 12 days.
  - A (GLP status not reported) biodegradation study was conducted under aerobic conditions using unadapted and adapted sludge. Propylene glycol reached 84-95% biodegradation within 24 hours and was reported as readily biodegradable.
- U.S. EPA 2012
  - BIOWIN predicted that propylene glycol is readily biodegradable. Fugacity modeling indicates that 65% will partition to soil with a half-life of 17 days, 34.5% will partition to water with a half-life of 8.7 days and 0.397% will partition to air with a half-life of 21.4 hours (Appendix D).
- While no studies following modern guidelines have been reported, the weight-of-evidence supports that propylene glycol is expected to be readily biodegradable.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
Propylene glycol was assigned a score of Very Low for bioaccumulation based on measured log K_{ow}. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when log K_{ow} values < 4 and/or BCF < 100(CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists.
- U.S. EPA 2012
  - A BCF of 0.8963 is estimated from the measured log K_{ow} of -0.92 (Appendix D)

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Propylene glycol was assigned a score of Low for reactivity based on NFPA reactivity score of 0 and expert judgment. Confidence level was reduced due to lack of experimental data. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when they are not explosive, and there is no evidence of them being reactive otherwise (CPA 2012a).

- Authoritative and Screening Lists
  - Not on any authoritative or screening lists

- NJDOH 2009
    - Propylene glycol has a NFPA reactivity score of 0 (stable: not reactive when mixed with water)
- Propylene glycol would not be classified as an oxidizing chemical as it structure does not contain a halogen and oxygen atoms present are only bonded to carbon or hydrogen (UN 2013). In addition, propylene glycol is not expected be explosive as it does not contain structural groups that would cause concern for explosion. Furthermore, the high flashpoint (103°C) further supports that propylene glycol is not a reactive chemical.

Flammability (F) Score (vH, H, M, or L): L

Propylene glycol was assigned a score of Low for flammability based on being not classifiable as a flammable liquid under GHS. GreenScreen® criteria classify chemicals as a Low hazard for flammability when not classified as flammable liquids (CPA 2012a).

- Authoritative and Screening Lists
    - Not on any authoritative or screening lists
- UNEP 2001
    - A flash point of 103°C was reported for propylene glycol. Following GHS criteria, propylene glycol is not classified as a flammable liquid (UN 2013).

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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 Propylene glycol (CAS #57-55-6)

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 / Propylene glycol / 57-55-6	L	L	M	*M*	DG	L	DG	*M*	M	DG	L	DG	L	L	L	L	vL	vL	*L*	L

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Propylene glycol	2

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

Table 6

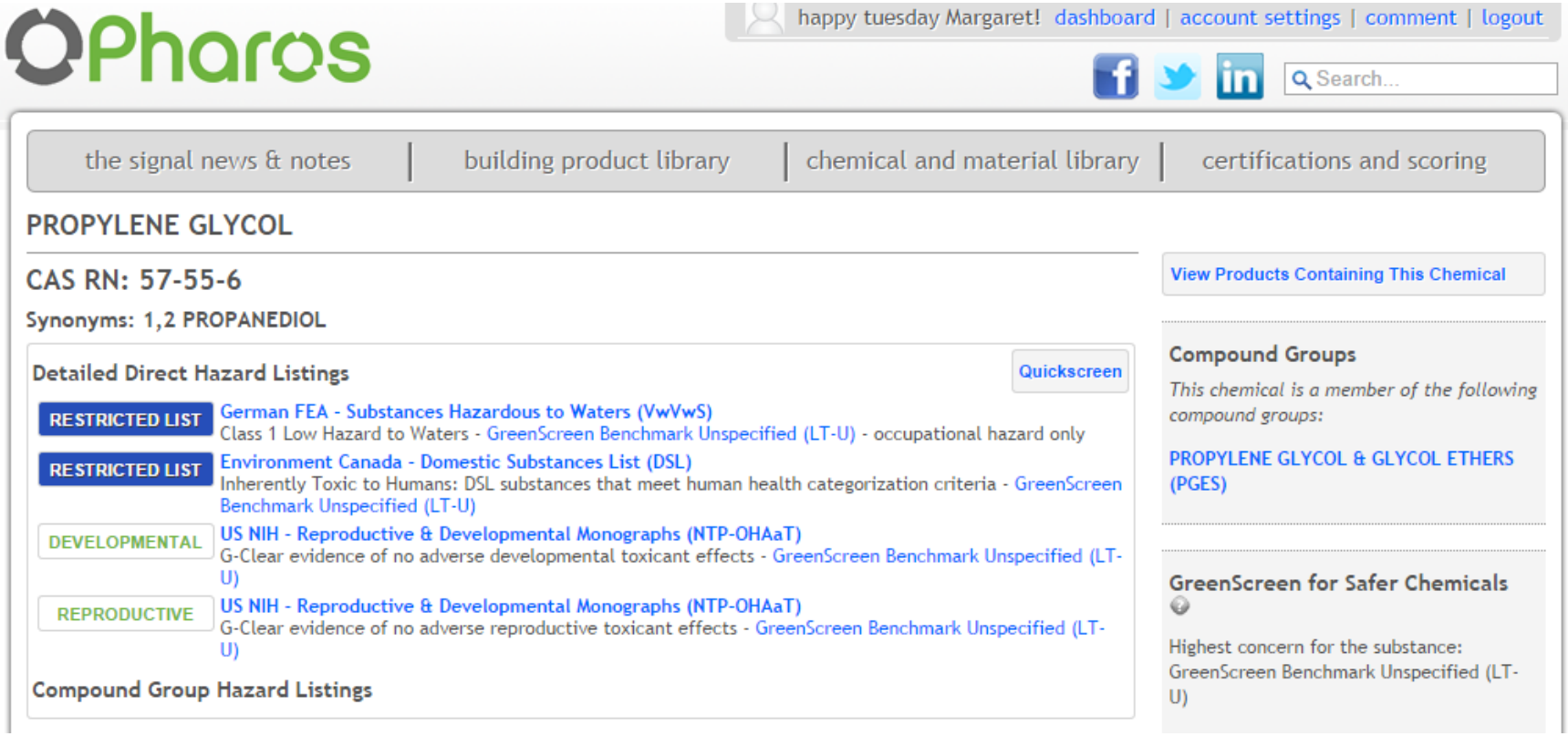
Chemical Name	Final GreenScreen® Benchmark Score
Propylene glycol	2

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												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for Propylene Glycol (CAS #57-55-6)



APPENDIX D: EPISuite Modeling Results for Propylene Glycol (CAS #57-55-6)

CAS Number: 57-55-6
SMILES: OCC(O)C
CHEM: 1,2-Propanediol
MOL FOR: C3 H8 O2
MOL WT: 76.10
---------- 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) = -0.78
Log K_{ow} (Exper. database match) = -0.92
Exper. Ref: HANSCH, C. ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 155.15 (Adapted Stein & Brown method)
Melting Pt (deg C): -33.01 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 0.111 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C): 14.8 (Mean VP of Antoine & Grain methods)
MP (exp database): -60 deg C
BP (exp database): 187.6 deg C
VP (exp database): 1.29E-01 mm Hg (1.72E+001 Pa) at 25 deg C

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 8.111e+005
log K_{ow} used: -0.92 (expK_{ow} database)
no-melting pt equation used
Water Sol (Exper. database match) = 1e+006 mg/L (20 deg C)
Exper. Ref: YALKOWSKY, S.H. & DANNENFELSER, R.M. (1992)

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: 1.74E-007 atm-m^3/mole (1.76E-002 Pa-m^3/mole)
Group Method: 1.31E-010 atm-m^3/mole (1.33E-005 Pa-m^3/mole)
Exper Database: 1.29E-08 atm-m^3/mole (1.31E-003 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: 1.370E-008 atm-m^3/mole (1.388E-003 Pa-m^3/mole)
VP: 0.111 mm Hg (source: MPBPVP)
WS: 8.11E+005 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: -0.92 (exp database)
Log K_{aw} used: -6.278 (exp database)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 5.358
Log K_{oa} (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 1.0288
Biowin2 (Non-Linear Model): 0.9847
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.3509 (days-weeks)
Biowin4 (Primary Survey Model): 3.9968 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.8072
Biowin6 (MITI Non-Linear Model): 0.9362
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.8822
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): 17.2 Pa (0.129 mm Hg)
Log K_{oa} (K_{oa}win est): 5.358
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model: 1.74E-007
Octanol/air (K_{oa}) model: 5.6E-008
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 6.3E-006
Mackay model: 1.4E-005
Octanol/air (K_{oa}) model: 4.48E-006

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 12.8199 E-12 cm^3/molecule-sec
Half-Life = 0.834 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 10.012 Hrs.
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
1.01E-005 (Junge-Pankow, Mackay avg)

4.48E-006 (K_{oa} 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}: 0.392 L/kg (K_{ow} method)
Log K_{oc}: -0.407 (K_{ow} method)
Experimental Log K_{oc}: 0.36 (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) = -2.0600 days (HL = 0.008709 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.048 (BCF = 0.8963)
Log BAF Arnot-Gobas method (upper trophic) = -0.048 (BAF = 0.8963)
log K_{ow} used: -0.92 (expK_{ow} database)

Volatilization from Water:
Henry LC: 1.29E-008 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 3.959E+004 hours (1650 days)
Half-Life from Model Lake: 4.32E+005 hours (1.8E+004 days)

Removal In Wastewater Treatment:
Total removal: 1.85 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.75 percent
Total to Air: 0.00 percent
(using 10000 hr. Bio P,A,S)

Removal In Wastewater Treatment:
Total removal: 92.06 percent
Total biodegradation: 91.72 percent
Total sludge adsorption: 0.33 percent
Total to Air: 0.00 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	0.397	21.4	1000
Water	34.5	208	1000
Soil	65	416	1000
Sediment	0.061	1.87e+003	0

Persistence Time: 364 hr.

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

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

Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

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

Licensed GreenScreen® Profilers

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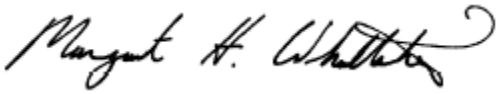

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