Method Version: GreenScreen® Version 1.2

Verified or Non-Verified: VERIFIED

Date of Verification:	**November 15 2013**
Expiration Date:	**November 15 2016**
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GreenScreen® Verification Performed By:	Clean Production Action
	Date: November 15 2013
	Verification Review Plan Prepared By: Dr. Eric Rosenblum
Verified GreenScreen® Prepared by Licensed Profiler:	Organization: ToxServices LLC
	Date: October 15, 2013

Propylene (CAS #115-07-1) GreenScreen® Assessment

Prepared for:

Clean Production Action

Date:

October 15, 2013 (Verified)

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GreenScreen® Executive Summary for Propylene (CAS #115-07-1)

Propylene is a major chemical intermediate in the chemical industry and in the production of a large range of chemicals

Propylene (gas) was assigned a GreenScreen® Benchmark Score of U ("Unspecified"). This chemical has High Flammability and High Reactivity (Appendix B), which corresponds to GreenScreen® benchmark classification 2g (High Flammability or High Reactivity) in CPA 2011a. Data gaps (dg) exist for Skin Irritation (IrS), Skin Sensitization (SnS*) and Respiratory Sensitization (SnR*). However, as outlined in CPA (2013) Section III (1) (Benchmarking Chemicals with Data Gaps), propylene fails the requirements for a GreenScreen® Benchmark Score of 2 due to data gaps. As a result, a Benchmark Score of U is assigned. In a worst-case scenario, if propylene were assigned a High score for these data gaps (Skin irritation, Skin and/or Respiratory Sensitization), it would be categorized as a Benchmark 2 Chemical and be classified as both 2f (Very High T or High T) and 2g (High Flammability or High Reactivity). Therefore, the highest and lowest possible Benchmark scores for propylene are both Benchmark 2.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
All exposure routes (oral, dermal and inhalation) were evaluated together, as a standard approach for GreenScreen® evaluations, so the GreenScreen® Benchmark Score of U ("Unspecified") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for Propylene

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

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

GreenScreen® Assessment for Propylene (CAS #115-07-1)

GreenScreen® Version 1.2 Assessment

Chemical Name: Propylene

CAS Number: 115-07-1

GreenScreen® Assessment Prepared By:
Name: Bingxuan Wang, Ph.D.

Title: Toxicologist
Organization: ToxServices LLC
Date: February 25, 2013 (Draft); May 29, 2013 (Revision #1)

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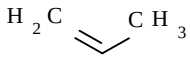
Title: Managing Director and Chief Toxicologist
Organization: ToxServices LLC
Date: April 11, 2013 (Draft); June 3, 2013 (Revision #1)

Confirm application of the *de minimus* rule[1]: N/A

Chemical Structure(s):



(CAS #115-07-1)

Also called:
Propene; 1-Propene; 1-Propylene; Methylethene; Methylethylene

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

In order to address the data gap for respiratory sensitization, U.S. EPA's Analog Identification Methodology (AIM) program was used. This program identified several volatile gases as potential surrogates based on chemical structure, but no respiratory sensitization data were available for these chemicals. The chemicals that were investigated are presented below:

Isoprene (CAS# 78-79-5); isobutene (115-11-7); 1,3-pentadiene (CAS# 504-60-9); 1,2-butadiene (CAS# 590-19-2); 1,3-dimethyl-1,3-butadiene (CAS# 1118-58-7); 2,3-dimethyl-1,3-butadiene (CAS# 513-81-5); hydrocarbons, C2-4 (CAS# 68606-25-7); 1-propene, 2-methyl-, homopolymer (CAS# 9003-27-4); 2-methylpropene (dimer) (CAS# 18923-87-0); 1,3-pentadiene, 4-methyl- (CAS# 926-56-7)

Notes related to production-specific attributes[2]: No information disclosed.

[1] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm

[2] Note any composition or hazard attributes of the chemical product relevant to how it is manufactured. For example, certain synthetic pathways or processes result in typical contaminants, by-products or transformation products. Explain any differences between the manufactured chemical product and the GreenScreen® assessment of the generic chemical by CAS #.

Identify Applications/Functional Uses:
1. Monomer and comonomer for polypropylene, ethylene-propylene elastomers and polymer gasoline for plastics and carpet fibers (HSDB 2011).
2. Chemical intermediate in the manufacture of acetone, isopropylbenzene, isopropanol, isopropyl halides, propylene oxide, acrylonitrile and cumene (HSDB 2011).
3. An aerosol propellant and component (HSDB 2011).

GreenScreen® Summary Rating for Propylene[3]: Propylene (gas) was assigned a GreenScreen® Benchmark Score of U ("Unspecified"). This chemical has High Flammability and High Reactivity (Appendix B), which corresponds to GreenScreen® benchmark classification 2g (High Flammability or High Reactivity) in CPA 2011a. Data gaps (dg) exist for Skin Irritation (IrS), Skin Sensitization (SnS*) and Respiratory Sensitization (SnR*). As outlined in CPA (2013) Section III (1) (Benchmarking Chemicals with Data Gaps), propylene fails the requirements for a GreenScreen® Benchmark Score of 2 due to data gaps. As a result, a Benchmark Score of U is assigned. In a worst-case scenario, if propylene were assigned a High score for these data gaps (Skin irritation, Skin and/or Respiratory Sensitization), it would be categorized as a Benchmark 2 Chemical and be classified as both 2f (Very High T or High T) and 2g (High Flammability or High Reactivity). Therefore, the highest and lowest possible Benchmark scores for propylene are both Benchmark 2.

Figure 1: GreenScreen® Hazard Ratings for Propylene

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

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 relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern[4,5]

Based on its molecular formula, possible combustion products of propylene are CO and CO_2. Although they are feasible environmental transformation products, they are not considered relevant to this GreenScreen® assessment, as they are naturally occurring in the environment, and are not persistent or bioaccumulative.

[3] 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.
[4] 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.
[5] The assessment of transformation products depends on the Benchmark Score of the parent chemical (see CPA Guidance 2013).

Introduction

Propylene in the environment results from natural and man-made sources. It is a natural product produced by vegetation. On the other hand, it is a combustion product from organic matter, motor vehicle exhaust, and cigarette smoke. Propylene is a major chemical intermediate in the chemical industry and in the production of a large range of chemicals (UNEP 2003).

ToxServices assessed Propylene against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.37 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results[6]

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2013) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for propylene can be found in Appendix B and a summary of the results can be found below:

- High hazard of flammability: EC - CLP/GHS Hazard Statements (EU H-Statements): H220 Extremely flammable gas.
- High hazard of flammability: Québec CSST - WHMIS Classifications (WHMIS): Class B1 - Flammable gases. High hazard of flammability:
- New Zealand HSNO/GHS (GHS-New Zealand): 2.1.1A - Flammable Gases: high hazard
- Intnl Agency for Rsrch on Cancer - Cancer Monographs (IARC): Group 3: Agent is not classifiable as to its carcinogenicity to humans

While Pharos searches most lists specified by the List Translator, it does not search DOT lists (U.S. DOT 2008a, b), that are required for a List Translator Screening Assessment. Therefore, these lists were searched manually:

This chemical did not appear on any of the above mentioned lists.

PhysioChemical Properties of Propylene

Propylene is a colorless gas at room temperature. It has moderate water solubility and is lighter than water.

Table 1: Physical and Chemical Properties of Propylene

Property	Value	Reference
Molecular formula	C3H6	HSDB 2011
SMILES Notation	C(C)=C	ChemIDplus 2013
Molecular weight	42.0804	ChemIDplus 2013
Physical state	Gas	HSDB 2011
Appearance	Colorless	HSDB 2011

[6] The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to screen for GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2013) is an online list-searching tool that is used to screen chemicals against the lists in the List Translator electronically.

Table 1: Physical and Chemical Properties of Propylene		
Property	**Value**	**Reference**
Melting point	-185℃	HSDB 2011
Vapor pressure	8.69 x 10^3 mm Hg at 25℃	HSDB 2011
Water solubility	200 mg/L at 25℃	HSDB 2011
Dissociation constant	N/A	
Density/specific gravity	0.5139 at 20℃/ 4℃ (liquid)	HSDB 2011
Partition coefficient	1.77	HSDB 2011

Hazard Classification Summary Section

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M or L): L
Propylene was assigned a score of L for carcinogenicity based on negative findings in rodent carcinogenicity studies. GreenScreen® criteria classify chemicals as a low hazard for carcinogenicity when adequate data are available and negative; the chemicals don't have structural alerts, and are not classified under GHS (CPA 2012a).

- HSDB 2011
  - IARC: there is inadequate evidence in humans and in experimental animals for the carcinogenicity of propylene. Propylene is not classifiable as to its carcinogenicity to humans (Group 3).
  - American Conference of Governmental Industrial Hygienists (ACGIH): A4 – not classifiable as a human carcinogen.
- UNEP 2003
  - No evidence of carcinogenicity was found in F344/N rats and B6C3F1 mice exposed to propylene by inhalation at concentrations of 5,000 or 10,000 ppm for 103 weeks. Propylene induced squamous metaplasia of the respiratory epithelium in male and female rats and epithelial hyperplasia in female rats, but more recent re-evaluation of this study revealed no dose-response for these effects.
- Based on the weight of evidence, propylene was assigned a score of low for carcinogenicity. It is not classifiable as to carcinogenicity, and carcinogenicity studies in both rats and mice were negative.

Mutagenicity/Genotoxicity (M) Score (H, M or L): L
Propylene was assigned a score of L for mutagenicity/genotoxicity based on mostly negative findings in gene mutation and chromosomal aberration tests. GreenScreen® criteria classify chemicals as a L hazard for mutagenicity/genotoxicity when adequate data are available and negative for both chromosomal aberrations and gene mutations, there are no structural alerts, and they are not GHS-classified (CPA 2012a).

- UNEP 2003
  - *In vitro bacteria reverse mutation assays*: Propylene has been tested in *Salmonella typhimurium* strains TA97, TA98, TA100, TA1535 and TA1537 and *Escherichia coli* strain WP2 uvrA (pKM101) at concentrations up to 10,000 ppm in the presence and absence of metabolic activation. Some mutagenic activity was only observed at

concentrations above 2,500 ppm in TA1535 in the presence of S9.
  - *In vitro mouse lymphoma assay:* No evidence of mutagenicity was observed at concentrations from 20 – 50% in the absence of S9, but in the presence of S9 equivocal results were obtained.
  - *In vivo micronucleus assay:* Male F344 rats were exposed to 200 – 10,000 ppm propylene by inhalation for 6 hours/day, 5 days/week for a total of 20 exposures. No increased micronucleus formation was found in bone marrow polychromatic erythrocytes.
  - *In vivo Hprt assay:* Male F344 rats were exposed to propylene at 200 – 10,000 ppm for 20 days. The trea®ents did not produce an increase in *Hprt* mutant frequencies in splenic T-lymphocytes.
- Although mutagenic activity was only seen in 1 of 5 bacterial strains tested in the Ames assay among many *in vivo* and *in vitro* assays of genotoxicity, the weight of evidence indicates that propylene is not genotoxic. The majority of *in vitro* mutagenicity studies in bacteria as well as an *in vivo* mutagenicity study in mice were negative. *In vivo* micronucleus tests and Hprt assays in rats were also negative.

Reproductive Toxicity (R) Score (H, M, or L): L
Propylene was assigned a score of L for reproductive toxicity based on negative findings in repeated dose inhalation toxicity studies. GreenScreen® criteria classify chemicals as a L hazard for reproductive toxicity when there are adequate and negative data available, chemicals have no structural alerts, and are not classified under GHS (CPA 2012a).
- U.S. EPA 2010
  - In the repeated dose inhalation toxicity studies in rodents (13 week study in F344 rats; 14 week study in $B6C3F_1$ mice; and 2 year study in F344 rats) described under Systemic Toxicity/Organ Effects (Repeated Exposure), no trea®ent-related histological effects were found in reproductive organs (mammary gland, seminal vesicles, prostate, testes, ovaries and uterus) in animals exposed to propylene for 14 and 103 weeks.
- Based on the weight of evidence, a score of low was assigned due to a lack of histological effects on reproductive organs in rats and mice.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M or L): L
Propylene was assigned a score of L for developmental toxicity based on negative findings in rats. GreenScreen® criteria classify chemicals as a L hazard for developmental toxicity when there are adequate and negative data available, chemicals have no structural alerts, and are not classified under GHS (CPA 2012a).
- U.S. EPA 2010
  - In a prenatal developmental toxicity study, pregnant Wistar rats (25/group) were exposed to propylene via whole-body inhalation at concentrations of 0, 200, 1,000, and 10,000 ppm for 6 hours/day on gestation days 6 – 19. There were no changes in food and water consumption, body weight, uterine weights or clinical and necropsy observations in dams. No maternal toxicity or developmental toxicities were observed on conception rate, mean number of corpea lutea, total implantations, pre/post-implantation losses or resorptions, the number of live fetuses, fetal sex ratio, fetal body weights, and external, soft tissue and skeletal abnormalities in the offspring. The NOAEC for maternal and developmental toxicity was 10,000 ppm, which is the highest concentration tested.
- Based on the weight of evidence, a score of low was assigned since no effects on a suite of developmental endpoints were observed in rats following gestational exposure.

Endocrine Activity (E) Score (H, M or L): *L*
Propylene was assigned a score of L for endocrine disruption based on the absence of endocrine disrupting activities in repeated dose inhalation toxicity studies in rodents. Confidence in this conclusion is low, as pathological examination does not represent a thorough evaluation of endocrine effects. GreenScreen® criteria classify chemicals as a L hazard for endocrine disruption when adequate negative data are available and chemicals don't have structural alerts (CPA 2012a).

- 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.
- ECHA 2013a
    - In the 2-year NTP inhalation toxicity studies in rats and mice described in the repeated dose toxicity section, histopathology was performed on the mammary gland, thymus, thyroid gland, parathyroid, pancreas, adrenal glands, reproductive organs and pituitary glands and no adverse effects were observed.
    - In the subchronic NTP inhalation toxicity studies in rats and mice described in the repeated dose toxicity section, gross pathology and histopathology were performed on the mammary gland, thymus, thyroid gland, parathyroid, pancreas, adrenal glands, reproductive organs and pituitary glands, and no adverse effects were noted.
- Based on the weight of evidence, no endocrine disrupting activity of propylene was observed as demonstrated by pathological examinations of multiple endocrine organs in repeated dose toxicity studies. However, these pathological evaluations merely suggest low potential for endocrine activity but do not represent a thorough evaluation of endocrine effects. Therefore confidence in this conclusion is low.

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 was assigned a score of L for acute toxicity based on 4h-inhalation LC_{50} of over 120 mg/L. GreenScreen® criteria classify chemicals as a L hazard for acute toxicity when 4h-inhalation LC_{50} values for gases are greater than 20 mg/L (CPA 2012a).

- U.S. EPA 2010
    - Inhalation LC_{50} (Sprague-Dawley rats, 4 hours) > 65,000 ppm or 120 mg/L[7]
    - Inhalation LC_{50} (male Sprague-Dawley rats, 4 hours) > 50,000 ppm or 92.5 mg/L[4]
- Propylene is a gas at ambient temperature and pressure and therefore ingestion or dermal absorption is unlikely. As a result, only acute inhalation toxicity studies were identified. Based on the weight of evidence, propylene is not an acute mammalian toxicant according to GHS classification based on inhalation LD_{50} values in rats.

[7] Conversion from ppm to mg/m^3 was performed using the website of Lenntech (http://www.lenntech.com/calculators/ppm/converter-parts-per-million.h®)

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)*(vH, H, M or L): L**
Propylene was assigned a score of L for systemic toxicity (single dose) based on animal data demonstrating a lack of systemic effects at doses > 10 mg/L. GreenScreen® criteria classify chemicals as a L hazard for systemic toxicity (single dose) when no systemic toxicity is observed below the guidance value of 10 mg/L for a gas inhalation study (CPA 2012a).

- UNEP 2003
    - Dogs could tolerate 50% (926 mg/L) propylene without apparent depression of circulation or respiration while lethal doses of propylene in dogs and cats were between 70 and 80% (1297 and 1482 mg/L).
    - 4-hour inhalation of 50,000 ppm (93 mg/L) propylene did not produce death or hepatotoxicity in Sprague-Dawley rats.
    - No signs of toxicity in cats (details not provided) was observed when anesthesia was maintained at propylene concentrations of 20 – 31% (371-574 mg/L). Some subtle effects were observed at concentrations of 40 – 50% and blood pressure decreases and rapid pulse occurred at a concentration of 70%. Unusual ventricular ectopic beat was observed with exposures from 50 – 80
- HSDB 2011
    - In 2 humans, propylene exposure at the concentrations of 35% and 40% caused vomiting during or after the experiment, and one complained of severe vertigo. Exposure to propylene at 40, 50 and 75% for a few minutes induced initial reddening of eyelids, flushing of face, lacrimation, coughing and sometimes flexing of legs.
- Based on the weight of evidence, a score of low was assigned. A rat study demonstrated a lack of hepatotoxicity at 93 mg/L for 4 hours. A dog study demonstrating a lack of effects on circulation and respiration at a dose of 926 mg/L, and a study in cats demonstrating no toxic effects at a dose of 371-574 mg/L support this classification. . Note: all conversions from ppm to mg/L were performed using the website of Lenntech (http://www.lenntech.com/calculators/ppm/converter-parts-per-million.h®)

***Group II* Score (repeated dose)* (H, M, or L): L**
Propylene was assigned a score of L for systemic toxicity (repeated dose) based on inhalation NOAELs of greater than 18.5 mg/L in rodents. GreenScreen® criteria classify chemicals as a L hazard for systemic toxicity (repeated dose) when effect levels are greater than 1 mg/L/6h/day for gases in inhalation toxicity studies (CPA 2012a).

- UNEP 2003 and U.S. EPA 2010
    - In a 13-week inhalation toxicity study performed by National Toxicology Program (NTP), F344 rats (9 – 11/sex/group) were exposed to propylene for 6 hours/day, 5 days/week at concentrations of 0, 625, 1,250, 2,500, 5,000 or 10,000 ppm in the air. Clinical observations and body weights were monitored during the study. No trea®ent-related death or clinical signs occurred during the study. No gross or microscopic pathologic effects (including reproductive organs and nasal cavity changes) were found upon necropsy. Exposed male rats had 4 – 12% higher mean body weights throughout most of the study while no differences in body weight gain was observed in females compared to controls. The mean body weight differences in males were determined not to be related to trea®ent. The no observed adverse effect level (NOAEL) was established at 10,000 ppm.
    - In a 14-week inhalation toxicity study performed by National Toxicology Program (NTP), $B6C3F_1$ mice (10/sex/group) were exposure to propylene for 6 hours/day, 5

days/week at concentrations of 0, 625, 1,250, 2,500, 5,000 or 10,000 ppm in the air. Clinical observations and body weights were monitored during the study. No gross or microscopic pathologic effects (including reproductive organs and nasal cavity changes) were found upon necropsy. In propylene-exposed females, a 4 – 7% decrease in final weight compared to controls was observed, but was determined not to be trea®ent related. The NOAEL was established at 10,000 ppm.

- In a 2-year inhalation toxicity study performed by National Toxicology Program (NTP), F344 rats (50/sex/group) were exposed to propylene for 6 hours/day, 5 days/week at concentrations of 0, 5,000 or 10,000 ppm in the air (98.6 – 99.7% pure) for 103 weeks. Survival was not affected by the trea®ent. Mean body weights of exposure animals were 0 – 5% lower than controls without dose-response relationships. No trea®ent-related adverse clinical signs, gross or microscopic lesions of the reproductive organs were observed. Upon histopathological examination, portal-of-entry effects of increased incidence of squamous metaplasia in both trea®ent groups and inflammation of the nasal cavities at 10,000 ppm were observed in females. These effects were not observed in animals exposed to similar concentrations for 14 weeks. The NOAEL was established at 10,000 ppm by U.S. EPA (2010) while the UNEP (2003) established the NOAEL at < 5,000 ppm based on increased squamous metaplasia and inflammation of the nasal cavities.
- In a 2-year inhalation toxicity study performed by National Toxicology Program (NTP), $B3C3F_1$ mice (50/sex/group) were exposed to propylene for 6 hours/day, 5 days/week at concentrations of 0, 5,000 or 10,000 ppm in the air (98.6 – 99.7% pure) for 103 weeks. Survival rates were not affected by propylene trea®ents. Slight decrease in mean body weights were observed at 10,000 ppm after week 59. No compound-related clinical signs, gross or microscopic lesions of the reproductive organs or nasal cavity were noted. NOAEL was established at 10,000 ppm.
- In a repeated dose biomarker/mutagenicity dose-response study in male F344 rats, animals (8/group) were exposed to propylene at concentrations of 0, 200, 2,000 or 10,000 ppm in the air for 6 hours/day for a total of 1, 3, or 20 exposures. The subgroup receiving 20 exposures included females as well. Sections of the nasal cavity of rats from all groups were microscopically examined and immunohistochemically prepared to identify nasal epithelial cells undergoing DNA synthesis. No propylene-related nasal lesions were microscopically detected in any groups. No exposure-related inflammation (rhinitis) or alterations were noted such as degeneration, necrosis, hyperplasia and metaplasia in the squamous, transitional, respiratory of olfactory epithelium lining in the nasal airways. No apparent exposure-related changes in the number of cells undergoing DNA synthesis were found in the nasal epithelium. No propylene exposure-related effects on cell proliferation were found in the liver or nasal respiratory epithelium. The NOAEL was established at 10,000 ppm both in males and females.

- Based on the weight of evidence, no adverse systemic effects occurred in rodents at propylene concentrations of 10,000 ppm (18.5 mg/L) in each of the repeated dose inhalation toxicity studies described above.

Neurotoxicity (N)

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

Propylene was assigned a score of M for neurotoxicity (single dose) based on GHS classification of Category 3 based on narcotic effects for specific target organ toxicity (single exposure).

GreenScreen® criteria classify chemicals as a M hazard for neurotoxicity (single dose) when they are classified as GHS Category 3 chemicals for Single Exposure target organ toxicity (CPA 2012a).

- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- UNEP 2003
    - In acute rodent inhalation studies, 30 – 40% (300,000 – 400,000 ppm) of propylene was minimally anesthetic
    - 37% propylene in oxygen or air induced narcosis in cats. 70% propylene induced anesthesia in cats within 2 minutes of exposure, but the animals recovered quickly with no apparent lasting effects. No signs of toxicity were observed when anesthesia was maintained at propylene concentrations of 20 – 31%. In conclusion, 40 – 50% propylene was narcotic to cats.
    - It has been estimated that narcotic concentration of propylene in humans is 46% (46,000 ppm), which is above the lower flammability level (20,000 ppm) for the chemical, meaning that the explosive range of airborne concentrations of propylene will be reached before any physiologic effects can be manifested.
- HSDB 2011
    - In humans, propylene exposure at the concentration of 6.4% (6,400 ppm or 11.8 mg/L[4]) for 2.25 minutes produced mild intoxication, paresthesia and inability to concentrate without memory impairment. Exposure at 12.8% for 1 minute induced the same but markedly accentuated symptoms. Exposures at 24% and 33% for 3 minutes caused unconsciousness. Exposure to 23% for 3 – 4 minutes did not produce unconsciousness.
    - In 2 humans, propylene exposure at the concentrations of 35% and 40% caused vomiting during or after the experiment, and one complained of severe vertigo. 50% propylene prompted anesthesia in two minutes followed by complete recovery without any physiological indications.
- Based on the weight of evidence, propylene can induce narcosis in humans at concentrations as low as 6.4 % (11.8 mg/L). However, these effects are reversible at concentrations up to 50% (92.5 mg/L). According to GHS classification criteria, propylene can be classified as a Category 3 chemical under specific target organ toxicity (single exposure).

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

Propylene was assigned a score of L for neurotoxicity (repeated dose) based on the lack of neurotoxicities in repeated dose toxicity studies at doses up to 10,000 ppm (18.5 mg/L). GreenScreen® criteria classify chemicals as a L hazard for neurotoxicity (repeated dose) when effect levels are greater than 1 mg/L/6h/day for gases according to GHS classification criteria for repeated dose toxicity studies (CPA 2012a).

- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- ECHA 2013a
    - In the 2-year NTP inhalation toxicity studies in rats and mice described in the repeated dose toxicity section, histopathology was performed on sternebrae, vertebrae, bone marrow, brain and spinal cord and no adverse effects were observed.
    - In the subchronic NTP inhalation toxicity studies in rats and mice described in the repeated dose toxicity section, gross pathology and histopathology were performed on sciatic nerve, sternebrae, vertebrae, bone marrow, brain and spinal cord, and no adverse effects were noted.
- Based on the weight of evidence, although neurobehavioral endpoints were not monitored in the repeated dose toxicity studies described above, gross pathological and histopathological

examinations on some neuronal tissues and organs did not reveal any adverse effects at propylene concentrations of up to 10,000 ppm in rodents.

Skin Sensitization (SnS) Group II* Score (H, M or L): DG
Propylene was assigned a score of DG for skin sensitization based on lack of data. GreenScreen® criteria classify chemicals as a DG hazard for skin sensitization when there are insufficient data available (CPA 2012a).

- No relevant data were identified.
- Surrogates for propylene were not investigated for propylene, as skin sensitization studies for a gas are not feasible. Therefore, this endpoint is a data gap.

Respiratory Sensitization (SnR) Group II* Score (H, M or L): DG
Propylene was assigned a score of DG for respiratory sensitization based on lack of data. GreenScreen® criteria classify chemicals as a DG hazard for respiratory sensitization when there are insufficient data available (CPA 2012a).

- No relevant data were identified for propylene.
- Several surrogates for propylene (identified above) were investigated, but no data on respiratory sensitization were available for these chemicals. Therefore respiratory sensitization remains a data gap.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M or L): DG
Propylene was assigned a score of DG for skin irritation/corrosivity based on lack of data. GreenScreen® criteria classify chemicals as a DG for skin irritation/corrosivity when there are insufficient data available (CPA 2012a).

- ESIS 2000
    - Although rapid evaporation of liquid propylene may freeze the skin and cause "frost bite", the gas produces little or no irritation in animals and humans.
- UNEP 2003
    - Two humans were anesthetized by 35 or 40% propylene without disagreeable sensations. Information about the route of exposure was not available.
- Surrogates for propylene (identified above) were investigated for skin irritation data. Data were identified for only one surrogate, isoprene (CAS #78-79-5), but the studies were not of sufficient quality to include in this assessment (assigned a Klimisch score of 4 (not assignable) in the REACH Dossier of isoprene) (ECHA 2013b). These studies were, therefore, not considered suitable to address the data gap for skin irritation for propylene.
- Based on the lack of available data, propylene gas is considered a data gap for skin irritation. Anecdotal evidence in two individuals did not specifically describe skin irritation or provide the route of exposure. Guideline studies for dermal irritation are not available for gases. Therefore, this endpoint is a data gap.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M or L): M
Propylene was assigned a score of M for eye irritation/corrosivity based on reported slight irritating effects in humans. GreenScreen® criteria classify chemicals as a M hazard for eye irritation/corrosivity when they are mild ocular irritants (CPA 2012a).

- UNEP 2003
    - In a human study, volunteers were exposed to mixtures of propylene (1 – 8 ppm) and nitric oxide (0 – 4 ppm). A reduction in propylene concentration led to a direct decline in eye irritation.

  - In another human study, a mixture of 1 ppm propylene and 0.25 ppm nitric oxide resulted in slight irritation, and when the propylene concentration increased to 2 – 3 ppm, moderate irritation was reported.
  - Two humans were anesthetized by 35 or 40% propylene without disagreeable sensations.
- Based on the weight of evidence, although inconsistent human experiences were reported, propylene may be slightly irritating to the eyes in humans. For substances that are considered mildly irritating to eyes, a GHS Category 2 classification, which corresponds to a score of moderate, is appropriate.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M or L): *M*
Propylene was assigned a score of M for acute aquatic toxicity based on predicted acute aquatic toxicity EC_{50} of 24.416 mg/L in green algae. GreenScreen® criteria classify chemicals as a M hazard for acute aquatic toxicity when L/EC_{50} values are between 10 and 100 mg/L (CPA 2012a).

- U.S. EPA 2012
  - No measured data are available and therefore ECOSAR was used to model the aquatic toxicity of propylene. This chemical is designated as the Neutral Organics chemical class with predicted L/EC_{50} values of 67.234 mg/L in fish (96h), 37.060 mg/L in daphnia (48h) and 24.416 mg/L in green algae. The most conservative acute aquatic toxicity value is therefore 24.416 mg/L in green algae (Appendix D).
- A score of moderate was assigned based on modeled data. Confidence in this conclusion is reduced due to the lack of experimental data for this endpoint. Propylene is highly volatile and will not remain in water for long periods of time.

Chronic Aquatic Toxicity (CA) Score (vH, H, M or L): *M*
Propylene was assigned a score of M for chronic aquatic toxicity based on predicted chronic toxicity value of 3.327 mg/L in daphnia. GreenScreen® criteria classify chemicals as a M hazard for chronic aquatic toxicity when guidance values are between 1.0 and 10 mg/L (CPA 2011c).

- U.S. EPA 2012
  - No measured data are available and therefore ECOSAR was used to model the aquatic toxicity of propylene. This chemical has predicted chronic values of 6.346 mg/L in fish, 3.327 mg/L in daphnia and 5.985 in green algae. The most conservative chronic value is therefore 3.327 mg/L in daphnia (Appendix D).
- A score of moderate was assigned based on modeled data. Confidence in this conclusion is reduced due to the lack of experimental data for this endpoint. Propylene is highly volatile and will not remain in water for long periods of time.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): L
Propylene was assigned a score of L for persistence based on its half-life in air. GreenScreen® criteria classify chemicals as a L hazard for persistence when half-life in air is < 2 days (CPA 2012a).

- UNEP 2003
  - Although no standard aquatic biodegradation tests were found for propylene because it presents severe technical challenges to achieving aqueous concentrations due to its potential to rapidly partition from water to air, it was scientifically judged to have aerobic, aqueous biodegradation half-life of between 7 and 28 days. There is also

sufficient information in the literature that demonstrates its potential to be metabolized by selected bacteria in the environment, although no information is available on the degradation rate.
    - Propylene will partition negligibly to the water compar®ent and the low levels in the water are unlikely to degrade by hydrolysis.
    - Propylene may degrade in soil but microbial degradation is likely to have little influence on the fate of propylene in the environment because propylene does not partition to soil.
    - Propylene is highly volatile and will partition predominantly to the a®osphere.
    - Propylene reacts readily with OH^- and O_3 in the air, and has half-lives between 15.1-23.8 hours based on reactions with OH^- and O_3, respectively.
- U.S. EPA 2011
    - BIOWIN predicts that propylene is readily biodegradable (Appendix E).
- Based on the weight of evidence, a score of low was assigned based on the half life of propylene in air. As propylene is highly volatile and partitions almost entirely to air, the half lives in water and soil are not relevant to the environmental fate of this substance. Therefore, only the measured half lives in air was considered for assigning the persistence score.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vL*
Propylene was assigned a score of vL for bioaccumulation based on estimated BCF of 5 and log K_{ow} of 1.77. GreenScreen® criteria classify chemicals as a vL hazard for bioaccumulation when BCF/BAF values are less than 5 and log K_{ow} values are less than 4 (CPA 2012a).
- HSDB 2011
    - An estimated BCF of 5 was calculated for propylene using a log K_{ow} of 1.77 and a regression-derived equation. This BCF suggests that the chemical has low potential for bioconcentration in aquatic organisms.
- U.S. EPA 2011
    - BCFBAF (EPISuite) predicted a BCF of 6.398 for propylene based on a measured log K_{ow} of 1.77 (Appendix E).
- A score of very low was assigned based on modeled data. Confidence in this conclusion is reduced due to the lack of experimental data for this endpoint.

<u>Physical Hazards (Physical)</u>

Reactivity (Rx) Score (vH, H, M or L): *H*
Propylene was assigned a score of H for reactivity based on classification into Division 1.3 for explosiveness according to GHS criteria. GreenScreen® criteria classify chemicals as a H hazard for reactivity when they are classified as GHS Division 1.1, 1.2 or 1.3 for explosiveness (CPA 2012a). Confidence in this conclusion is reduced because it is not based on the UN Test series recommended by GHS for classification.
- ICSC 1998
    - Gas/air mixtures of propylene are explosive.
- HSDB 2011
    - Propylene is explosive in the form of vapor when exposed to heat or flame. Under unusual conditions (i.e. 955 a® pressure and 327℃), it has been known to explode.
    - Lower explosive limit: 2.4%; upper explosive limit: 10.1%
    - Liquid propylene will explode on contact with water at 42-75 °C.
    - Cylinders exposed to fire may vent and release flammable gas. Containers may explode when heated. Ruptured cylinders may rocket.

- Based on the weight of evidence, propylene can be classified to Division 1.3 for explosiveness according to GHS criteria: "substance with a fire hazard and either a minor blast hazard or a minor projection hazard or both, but not a mass explosion hazard: (i): combustion of which gives rise to considerable radiant heat; or (ii) which burn one after another, producing minor blast or projection effects or both". HSDB reports that containers may explode when heated which indicates that the reaction is not confined to the package. Therefore Division 1.3, which corresponds to a high hazard, is appropriate. Confidence in this conclusion is reduced because it is not based on the UN Test series recommended by GHS for classification. No measured data are available for explosiveness or any reactivity endpoint.

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

Propylene was assigned a score of H for flammability based on association with EU Hazard Phrase of H220. GreenScreen® criteria classify chemicals as a H hazard for flammability when they are associated with H220 (CPA 2011c).

- Pharos 2013
    - Propylene is associated with EU Hazard Risk of H220: Extremely flammable gas.

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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

(Cr) Corrosion/ Irritation (Skin/ Eye)

(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

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	115-07-1	**L**	**L**	**L**	**L**	*L*	**L**	**L**	**L**	**M**	**L**	DG	DG	*DG*	**M**	*M*	*M*	**L**	*vL*	*H*	**H**

Table 3a: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen™ Benchmark Score
Propylene	2

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

Table 6

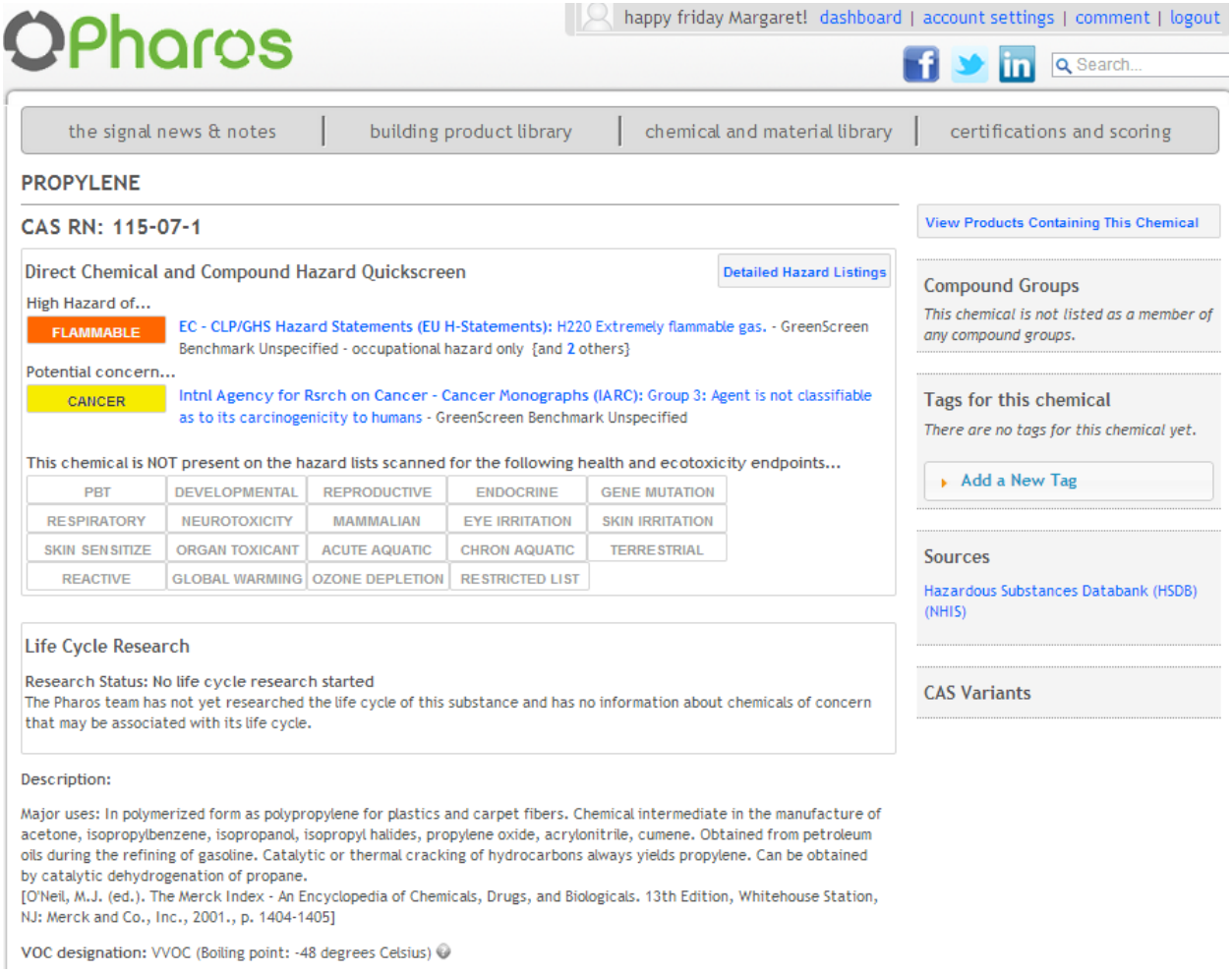
Chemical Name	Final GreenScreen™ Benchmark Score
Propylene	U

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	No	Yes	Yes	Yes							U
3												
4												

APPENDIX C: Pharos Output for Propylene



Pharos

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PROPYLENE

CAS RN: 115-07-1

View Products Containing This Chemical

Direct Chemical and Compound Hazard Quickscreen

Detailed Hazard Listings

High Hazard of...

FLAMMABLE — EC - CLP/GHS Hazard Statements (EU H-Statements): H220 Extremely flammable gas. - GreenScreen Benchmark Unspecified - occupational hazard only [and 2 others]

Potential concern...

CANCER — Intnl Agency for Rsrch on Cancer - Cancer Monographs (IARC): Group 3: Agent is not classifiable as to its carcinogenicity to humans - GreenScreen Benchmark Unspecified

This chemical is NOT present on the hazard lists scanned for the following health and ecotoxicity endpoints...

PBT	DEVELOPMENTAL	REPRODUCTIVE	ENDOCRINE	GENE MUTATION
RESPIRATORY	NEUROTOXICITY	MAMMALIAN	EYE IRRITATION	SKIN IRRITATION
SKIN SENSITIZE	ORGAN TOXICANT	ACUTE AQUATIC	CHRON AQUATIC	TERRESTRIAL
REACTIVE	GLOBAL WARMING	OZONE DEPLETION	RESTRICTED LIST	

Life Cycle Research

Research Status: No life cycle research started
The Pharos team has not yet researched the life cycle of this substance and has no information about chemicals of concern that may be associated with its life cycle.

Description:

Major uses: In polymerized form as polypropylene for plastics and carpet fibers. Chemical intermediate in the manufacture of acetone, isopropylbenzene, isopropanol, isopropyl halides, propylene oxide, acrylonitrile, cumene. Obtained from petroleum oils during the refining of gasoline. Catalytic or thermal cracking of hydrocarbons always yields propylene. Can be obtained by catalytic dehydrogenation of propane.
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1404-1405]

VOC designation: VVOC (Boiling point: -48 degrees Celsius)

Compound Groups

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

Tags for this chemical

There are no tags for this chemical yet.

Add a New Tag

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants

APPENDIX D: ECOSAR Output for Propylene

ECOSAR Version 1.11 Results Page

SMILES : C(=C)C
CHEM : 1-Propene
CAS Num: 000115-07-1
ChemID1:
MOL FOR: C3 H6
MOL WT : 42.08
Log Kow: 1.678 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: 1.77 (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: -185.00 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 1109 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: 200 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 1.678 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 200 (mg/L, PhysProp DB exp value)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	67.237
Neutral Organics	: Daphnid	48-hr	LC50	37.060
Neutral Organics	: Green Algae	96-hr	EC50	24.416
Neutral Organics	: Fish		ChV	6.346
Neutral Organics	: Daphnid		ChV	3.327
Neutral Organics	: Green Algae		ChV	5.985
Neutral Organics	: Fish (SW)	96-hr	LC50	84.483
Neutral Organics	: Mysid	96-hr	LC50	78.076

Neutral Organics	: Fish (SW)		ChV	7.535
Neutral Organics	: Mysid (SW)		ChV	7.424
Neutral Organics	: Earthworm	14-day	LC50	79.004

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 LogKow Cut-Offs

If the log Kow 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 LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

APPENDIX E: EPISuite Output for Propylene

CAS Number: 115-07-1
SMILES : C(=C)C
CHEM : 1-Propene
MOL FOR: C3 H6
MOL WT : 42.08
---------- EPI SUMMARY (v4.10) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (a®-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = 1.68
Log Kow (Exper. database match) = 1.77
Exper. Ref: HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): -9.84 (Adapted Stein & Brown method)
Melting Pt (deg C): -135.38 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 7.04E+003 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C) : 9.39E+005 (Mean VP of Antoine & Grain methods)
MP (exp database): -185 deg C
BP (exp database): -48 deg C
VP (exp database): 8.69E+03 mm Hg (1.16E+006 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 1162
log Kow used: 1.77 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 200 mg/L (25 deg C)
Exper. Ref: MCAULIFFE,C (1966)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 717.99 mg/L

ECOSAR Class Program (ECOSAR v1.00):
Class(es) found: Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 1.53E-001 a®-m3/mole (1.55E+004 Pa-m3/mole)
Group Method: 1.58E-001 a®-m3/mole (1.60E+004 Pa-m3/mole)
Exper Database: 1.96E-01 a®-m3/mole (1.99E+004 Pa-m3/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: 3.621E-002 a®-m3/mole (3.669E+003 Pa-m3/mole)
VP: 7.04E+003 mm Hg (source: MPBPVP)
WS: 1.16E+003 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 1.77 (exp database)
Log Kaw used: 0.904 (exp database)
Log Koa (KOAWIN v1.10 estimate): 0.866
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7275
Biowin2 (Non-Linear Model) : 0.9177
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.1062 (weeks)
Biowin4 (Primary Survey Model) : 3.7870 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.6059
Biowin6 (MITI Non-Linear Model): 0.8047
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5359
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days) : 0.3730
BioHC Half-Life (days) : 2.3603

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 1.16E+006 Pa (8.69E+003 mm Hg)
Log Koa (Koawin est): 0.866
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 2.59E-012
Octanol/air (Koa) model: 1.8E-012
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 9.35E-011
Mackay model : 2.07E-010
Octanol/air (Koa) model: 1.44E-010

A®ospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 26.4360 E-12 cm3/molecule-sec
Half-Life = 0.405 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 4.855 Hrs
Ozone Reaction:
OVERALL Ozone Rate Constant = 1.200000 E-17 cm3/molecule-sec
Half-Life = 0.955 Days (at 7E11 mol/cm3)
Half-Life = 22.920 Hrs

Fraction sorbed to airborne particulates (phi):
1.5E-010 (Junge-Pankow, Mackay avg)
1.44E-010 (Koa method)
Note: the sorbed fraction may be resistant to a®ospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 21.73 L/kg (MCI method)
Log Koc: 1.337 (MCI method)
Koc : 34.34 L/kg (Kow method)
Log Koc: 1.536 (Kow method)

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

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.835 (BCF = 6.837 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -0.5593 days (HL = 0.2758 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.806 (BCF = 6.398)
Log BAF Arnot-Gobas method (upper trophic) = 0.806 (BAF = 6.398)
log Kow used: 1.77 (expkow database)

Volatilization from Water:
Henry LC: 0.196 a®-m3/mole (Henry experimental database)
Half-Life from Model River: 0.6639 hours (39.83 min)
Half-Life from Model Lake : 61.64 hours (2.568 days)

Removal In Wastewater Trea®ent (recommended maximum 95%):
Total removal: 98.70 percent
Total biodegradation: 0.02 percent
Total sludge adsorption: 0.41 percent
Total to Air: 98.27 percent
(using 10000 hr Bio P,A,S)

Removal In Wastewater Trea®ent (recommended maximum 95%):
Total removal: 99.22 percent
Total biodegradation: 22.88 percent
Total sludge adsorption: 0.34 percent
Total to Air: 76.00 percent
(using Biowin/EPA draft method)

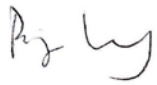
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	10.7	6.97	1000
Water	87.7	360	1000
Soil	1.44	720	1000
Sediment	0.24	3.24e+003	0

Persistence Time: 70.2 hr

Authorized Reviewers

Propylene GreenScreen® Evaluation Prepared By:



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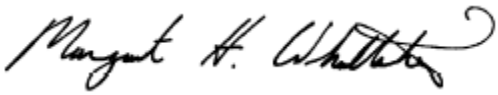
ToxServices LLC

Propylene GreenScreen® Evaluation QC'd By:



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