Propanol (CAS# 71-23-8) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

ToxServices LLC

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GreenScreen® Executive Summary for Propanol (CAS #71-23-8)

Propanol is a chemical that functions as a used as a flavoring substance in foods, as a solvent in inks, paint, cosmetics, and pesticides, as a chemical intermediate for the production of esters, amines, and other organic derivatives.

Propanol 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), Very High Group II Human Toxicity (eye irritation-IrE), and High Flammability-F. This corresponds to GreenScreen® benchmark classifications 2e, 2f and 2g in CPA 2011. Data gaps (DG) exist for endocrine activity-E, neurotoxicity-Ns*, and respiratory sensitization-SnR*. As outlined in CPA (2013) Section 12.2 (Conduct a Data Gap Analysis to assign a final Benchmark score), propanol meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if propanol 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 Propanol

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

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

GreenScreen® Assessment for Propanol (CAS #71-23-8)

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

Chemical Name: Propanol

CAS Number: 71-23-8

GreenScreen® Assessment Prepared By:
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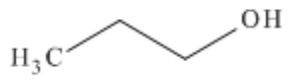
Title: Toxicologist
Organization: ToxServices LLC
Date: October 14, 2014
Assessor Type: Licensed GreenScreen® Profiler

Quality Control Performed By:
Name: Bingxuan Wang, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: December 1, 2014

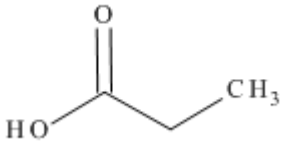
Confirm application of the *de minimus* rule[3]: N/A

Chemical Structure(s):



Also called: 1-Propanol; n-Propanol; n-Propyl alcohol; 1-Hydroxypropane; 1-Propyl alcohol; Ethyl carbinol; Ethylcarbinol; n-Propan-1-ol; Propanol-1; Propylic alcohol (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
A limited dataset was available for propanol. As it is readily metabolized to propionic acid (CAS# 79-09-4) i*n vivo*, this metabolite was used to fill data gaps for human toxicity endpoints.



Propionic acid (CAS# 79-09-4)

Identify Applications/Functional Uses:
1. Flavoring substance in foods
2. Solvent in inks, paint, cosmetics, and pesticides
3. Chemical intermediate for production of esters, amines, and organic derivatives (U.S. EPA 2005)

GreenScreen® Summary Rating for Propanol[4]: Propanol was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Moderate Group I Human Toxicity

[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

(reproductive toxicity-R and developmental toxicity-D), Very High Group II Human Toxicity (eye irritation-IrE), and High Flammability-F. This corresponds to GreenScreen® benchmark classifications 2e, 2f and 2g in CPA 2011. Data gaps (DG) exist for endocrine activity-E, neurotoxicity-Ns*, and respiratory sensitization-SnR*. As outlined in CPA (2013) Section 12.2 (Conduct a Data Gap Analysis to assign a final Benchmark score), propanol meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if propanol 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 Propanol

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**	**M**	**L**	**M**	DG	**L**	DG	**L**	**vH**	**L**	**L**	**vL**	**vL**	*L*	**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 feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

Since propanol is readily biodegradable, meeting the 10-day window (ECHA 2014a, see Persistence, below), it is not expected to produce any relevant transformation products.

Introduction

Propanol is naturally occurring in fossil fuels and as a fermentation and decomposition product of fruits and vegetables. It is used as a flavoring substance in foods, as a solvent in inks, paint, cosmetics, and pesticides, as a chemical intermediate for the production of esters, amines, and other organic derivatives (U.S. EPA 2005).

ToxServices assessed propanol against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.69 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation

[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.

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

Carcinogenicity
- Japan METI/MOE - GHS Classifications (GHS-Japan) Carcinogenicity Category 2

Reproductive Toxicity
- Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 2

Mammalian Toxicity
- New Zealand HSNO/GHS (GHS-New Zealand) 6.1D (oral) - Acutely toxic (Category 4)
- New Zealand HSNO/GHS (GHS-New Zealand) 6.1E (dermal) - Acutely toxic (Category 5)
- Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (oral) - Category 5
- Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (dermal) - Category 5
- Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 3
- Québec CSST - WHMIS Classifications (WHMIS) Class D2B - Toxic material causing other toxic effects

Neurotoxicity
- EC - CLP/GHS Hazard Statements (EU H-Statements) H336 May cause drowsiness or dizziness
- EC - Risk Phrases (EU R-Phrases) R67: Vapors may cause drowsiness and dizziness
- Patty's Toxicology - Boyes Neurotoxicants (Boyes-N) Neurotoxic

Skin Irritation
- Japan METI/MOE - GHS Classifications (GHS-Japan) Skin corrosion / irritation - Category 2

Eye Irritation
- EC - CLP/GHS Hazard Statements (EU H-Statements) H318 Causes serious eye damage
- EC - Risk Phrases (EU R-Phrases) R41: Risk of serious damage to eyes
- New Zealand HSNO/GHS (GHS-New Zealand) 6.4A - Irritating to the eye (Category 2A)
- Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2A

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

Other
- German FEA - Substances Hazardous to Waters (VwVwS) Class 1 Low Hazard to Waters
- Environment Canada - Domestic Substances List (DSL) Inherently Toxic to Humans: DSL substances that meet human health categorization criteria

PhysicoChemical Properties of Propanol

Propanol is a liquid at room temperature. It has a high vapor pressure of 21 mmHg, indicating that it is likely to form a gas. It is highly soluble in water (1×10^6 mg/L) and its log K_{ow} of 0.25 indicates that it has low bioaccumulation potential.

Table 1: Physical and Chemical Properties of Propanol (CAS #71-23-8)		
Property	**Value**	**Reference**
Molecular formula	C3-H8-O	ChemIDplus 2014
SMILES Notation	C(CO)C	ChemIDplus 2014
Molecular weight	60.0952	ChemIDplus 2014
Physical state	Liquid	U.S. EPA 2005
Appearance	Clear, colorless	U.S. EPA 2005
Melting point	-126°C	ChemIDplus 2014
Vapor pressure	21 mmHg at 25°C	ChemIDplus 2014
Water solubility	1 x 10^6 mg/L at 25°C	ChemIDplus 2014
Dissociation constant	pKa = 16.1	ChemIDplus 2014
Density/specific gravity	0.8	U.S. EPA 2005
Partition coefficient	log K_{ow} = 0.25	ChemIDplus 2014

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

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

Propanol was assigned a score of Low for carcinogenicity based on a lifetime carcinogenicity study of the metabolite propionic acid. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate data are available and are negative for carcinogenicity, and the chemical is not present on authoritative or screening lists (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Japan METI/MOE-GHS Classifications (GHS-Japan) Carcinogenicity Category 2

Propanol (CAS# 71-23-8)

- EU 2008
  - In a carcinogenicity study that was classified as invalid, 18 Wistar rats (males and females) were administered 240 mg/kg propanol via gavage twice weekly for a lifetime. Mean survival times in the treated and control rats were 570 and 643 days, respectively. Liver congestion, steatosis, necrosis, fibrosis, and extramedullary and medullary hyperplasia of the hematopoietic bone marrow parenchyma were seen in nearly all rats but incidence was not reported. Incidence of malignant tumors of the liver and bone marrow and of overall tumors was increased in treated animals. Because genotoxicity data are negative, other modes of action including hepatotoxicity should be considered. This study was considered to be inadequate for the EU risk assessment due to small sample sizes, unclear sex ratio, lack of detail about type of liver sarcomas, and lack of statistical analysis.
  - In a lifetime carcinogenicity study in male CH3 mice, animals were dermally administered 40 mg propanol 3 times/week. No skin tumors were seen. This study was considered to be inadequate for the EU risk assessment due to small sample sizes, use of only males, age of animals, different age control and test group, arbitrary locations for histopathology, and inadequate reporting.
  - There are no valid carcinogenicity studies available for propanol. Carcinogenicity is not considered to be a concern due to negative mutagenicity data.

Propionic acid (CAS# 79-09-4)

- ECHA 2014b

  - In a lifetime feeding study in male Wistar rats, animals (30/dose) were administered 0, 0.4, or 4% propionic acid (0, 264, or 2,640 mg/kg/day, purity not reported) in the diet for a lifetime. At necropsy, button-like hyperplastic ulcers with peripheral papillomatous protrusions/elevations (papillomas) were seen in almost all animals at the high dose. In 5 animals, precancerous sites that could eventually develop to squamous epithelial carcinomas were seen. Downward basal cell proliferation (hyperplasia) leading to downward basal cell proliferation (hyperplasia), large cysts in the wall of the stomach, and dysplasia of glandular stomach mucosa were also seen. Authors considered changes to be small local carcinomatous or precancerous transformations, but noted that although they may be early stages of tumor development, they are not regarded as preneoplastic in the current study due to the lack of tumors during the long study period. Authors also reported that changes are the result of chronic irritation and inflammation and the associated hyperplastic proliferative repair response. Authors identified a NOAEL of 2,640 mg/kg/day, and noted that the hyperplastic changes are a precursor for the development of local benign tumors and are not progressive

- Based on the weight of evidence, a score of Low was assigned. No adequate data are available for propanol, but negative genotoxicity results indicate that it is not likely to be a genotoxic carcinogen. In a study of propionic acid, precursors of benign tumors developed as a result of local irritation in the forestomach, but were found to be not progressive. Therefore a score of Low was assigned. Confidence in this score is reduced because there are no adequate studies available for propanol, and the study of propionic acid did not report data on tissues other than the forestomach.

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

Propanol was assigned a score of Low for mutagenicity/genotoxicity based on negative results in GLP-compliant *in vitro* bacterial and mammalian cell mutagenicity assays and an *in vitro* mammalian cell chromosome aberration assay. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when adequate data are available and are negative for both chromosomal aberrations and gene mutations, and the chemical is not present on authoritative or screening lists (CPA 2012a).

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

<u>Propanol (CAS# 71-23-8)</u>

- ECHA 2014a
  - Propanol (99.995% purity) was negative in a GLP-compliant mammalian cell gene mutation assay according to OECD Guideline 476 in Chinese hamster Ovary (CHO) cells when tested at concentrations up to 600 µg/mL (limit concentration) with and without metabolic activation. No mutagenicity was seen at any dose.
  - Propanol (99.82% purity) was negative in a GLP-compliant mammalian cell chromosome aberration test according to OECD Guideline 473 in Chinese hamster lung fibroblasts (V79) when tested at concentrations up to 600 µg/mL (limit concentration) with and without metabolic activation. There were no treatment related effects on chromosome aberrations.
  - Propanol (99.95% purity) was negative in a GLP-compliant bacterial reverse mutation assay according to OECD Guideline 471 in *S. typhimurium* strains TA1535, TA1537, TA98 and TA100 and *E. coli* WP2 uvr A when tested at concentrations up to 5000 µg/plate with and without metabolic activation. There was no increase in revertants at any dose in any strain.

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

Propanol was assigned a score of Moderate for reproductive toxicity based reversible effects on male fertility at a high inhalation concentration. 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
  - *Authoritative:* Not present on any authoritative lists
  - *Screening*: Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 2

Propanol (CAS# 71-23-8)

- NITE 1996
  - Propanol was classified as GHS Category 2 in Japan based on reproductive impairments in male rats and malformations (crooked tail) in offspring of female rats that were treated with inhalation doses that produced general toxicity.
- ECHA 2014a
  - In an inhalation 1-generation study of male reproductive toxicity in Sprague-Dawley rats, animals (18 males/dose, 15 sham females/dose) were administered 0; 3,500 or 7,000 ppm (0; 8,730 or 17,460 mg/m³ or 0, 8.73, or 17.46 mg/L[6]) propanol (>99% purity) via whole body inhalation for 7 hours/day, 7 days/week for 42 days prior to mating. Females were sham exposed on gestation days 1-19. A second experiment by the same authors in which females were administered the same doses on gestation days 1-19 is described below for developmental toxicity. Infertility was seen in males that were exposed to the high dose prior to mating, with only 2 litters of 12 and 2 pups were produced from 16 successful matings (based on sperm plugs). Due to the infertility, authors retained and remated 6 males from the high dose group at biweekly intervals. The number of males producing litters at weeks 1, 2, 5, 7, 11, 13, and 15 were 1, 2, 4, 4, 3, 6, and 6, respectively. Authors concluded that propanol produces reversible effects on male fertility at high doses, and identified a NOAEC of 8.73 mg/L.
- Based on the weight of evidence, a score of Moderate was assigned. Reversible effects on male fertility on which GHS classification in Japan was based were seen only at a relatively high inhalation dose (17.46 mg/L), with a NOAEC of 8.73 mg/L. Per GHS Guidance, adverse effects seen only at very high dose levels in animal studies are not normally sufficient for classification, unless available data indicate that humans are more susceptible than animals. No data were available regarding whether systemic toxicity was observed at these doses. Therefore, ToxServices conservatively assigned a Moderate score for this endpoint. Confidence level is reduced due to uncertainty regarding whether the fertility effect was secondary to systemic toxicity.

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

Propanol was assigned a score of Moderate for developmental toxicity based on inhalation toxicity studies in rats at a relatively high concentration. GreenScreen® criteria classify chemicals as a Moderate hazard for developmental toxicity when there is limited or marginal evidence in animals (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening*: Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 2
- NITE 1996

[6] 8,730 mg/m^3 * 1 m^3/1,000 L = 8.73 mg/L

  - Propanol was classified as GHS Category 2 in Japan based on reproductive impairments in male rats and malformations (crooked tail) in offspring of female rats that were treated with inhalation doses that produced general toxicity.

Propanol (CAS# 71-23-8)

- ECHA 2014a
  - In an inhalation toxicity study in Sprague-Dawley rats, untreated females (15/dose) were mated with untreated males and were then administered 3,500 or 7,000 ppm (0; 8,730 or 17,460 mg/m³ or 0, 8.73, or 17.46 mg/L) propanol (>99% purity) via whole body inhalation for 7 hours/day on gestation days 1-19. There was no evidence of teratogenicity at the low dose. At the high dose, 2/15 litters had several pups with crooked tails that persisted after birth. In an optical activity monitor, male offspring had significantly reduced activity than controls, but there were no effects on an open field test or activity wheel at this dose. There were no effects on any behavioral endpoint at the high dose. There were no neurochemical effects on offspring. ToxServices identified a NOAEC of 8.73 mg/L for developmental toxicity.
  - In an inhalation developmental toxicity study in Sprague-Dawley rats, dams (15/dose) were administered 0; 3,500, 7,000, or 10,000 ppm (0; 8,730, 17,460, or 24,940 mg/m³ or 0, 8.73, 17.46, or 24.94 mg/L) propanol (102.1% analytical purity) via whole body inhalation for 7 hours/day on gestation days 1-19. Maternal toxicity (reduced feed intake and reduced maternal body weight) was seen at the mid and high doses. At the mid and high doses, the incidence of skeletal malformations was significantly increased. Visceral malformations were also increased at the high dose. The incidence of resorptions was increased and incidence of live implants/litter was significantly decreased at this dose. Authors identified a NOAEC of 8.73 mg/L for both maternal toxicity and developmental toxicity.
- Based on the weight of evidence, a score of Moderate was assigned. GHS classification was based on teratogenicity (crooked tail) in offspring of females that were treated with high doses that caused general toxicity. In two inhalation toxicity studies, no effects on offspring development were seen at a dose of 8.73 mg/L.

Endocrine Activity (E) Score (H, M, or L): DG

Propanol was assigned a score of Data Gap for endocrine disruption based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening*: Not present on any screening lists
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.

Propanol (CAS# 71-23-8)

- High Throughput Screening (HTS) Data –
  - HTS data were identified for propanol using PubChem (http://pubchem.ncbi.nlm.nih.gov/).
  - The data included the following results:
    - Propanol was active in 0/3 androgen receptor agonist assays and 0/6 androgen receptor antagonist assays.
    - Propanol was active in 0/3 estrogen receptor-alpha agonist assays and 0/6 estrogen receptor-alpha antagonist assays.
    - Propanol was active in 0/1 thyroid receptor agonist assays and 0/3 thyroid receptor antagonist assays.

        - The activity of propanol towards the thyroid stimulating hormone receptor was not evaluated.
- These data are insufficient to assign a score for endocrine activity.

Propionic acid (CAS# 79-09-4)

- No data were identified.

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

Propanol was assigned a score of Low for acute toxicity based on acute oral, dermal, and inhalation LD/LC_{50} values in rats, mice, and rabbits. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral and dermal LD_{50} values are greater than 2,000 mg/kg and inhalation LC_{50} values are greater than 20 mg/L (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.1D (oral) - Acutely toxic (Category 4)
    - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.1E (dermal) - Acutely toxic (Category 5)
    - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (oral) - Category 5
    - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (dermal) - Category 5

Propanol (CAS# 71-23-8)

- ECHA 2014a
    - *Oral*: LD_{50} (rat, male, strain not specified) = 5,400 mg/kg.
    - *Oral*: LD_{50} (rat, male and female Osborne-Mendel) = 6,500 mg/kg.
    - *Oral*: LD_{50} (rat, sex not specified, Carworth-Wistar) = 1,870 mg/kg.
    - *Oral*: LD_{50} (rat, male and female Sprague-Dawley) = 8,000 mg/kg.
    - *Inhalation*: LC_{50} (rat, male and female Sprague-Dawley) > 33.8 mg/L/4h
    - *Inhalation*: LC_{50} (rat, male and female Wistar) > 51.91 mg/L/8h
    - *Inhalation*: LC_{50} (rat, male and female Wistar) > 62.48 mg/L/3h
    - *Inhalation*: LC_{50} (rat, male and female Sprague-Dawley) > 26.76 mg/L/7h
    - *Dermal:* LD_{50} (rabbit, male New Zealand White) = 4,032 mg/kg
    - *Dermal:* LD_{50} (rabbit, male, strain not specified) = 6,730 mg/kg
- EU 2008
    - *Oral*: LD_{50} values include 1,870, 6,500, and 8,000 mg/kg in rats, 2,823 mg/kg in rat, and 5,467 mg/kg in mouse. The Institute for Health and Consumer Protection of the European Chemicals Bureau concluded that these data do not warrant classification for acute oral toxicity.
    - *Inhalation*: The LC_{50} value is estimated to be 42.0 mg/L/4h. In two 8-hour inhalation studies there were 1/12 and 0/12 mortalities at a concentration of 47.0 mg/L. The Institute for Health and Consumer Protection of the European Chemicals Bureau concluded that these

data do not warrant classification for acute inhalation toxicity.
    - *Dermal*: The dermal LD_{50} value in rabbits is 4,052 mg/kg. The Institute for Health and Consumer Protection of the European Chemicals Bureau concluded that these data do not warrant classification for acute dermal toxicity.
- Based on the weight of evidence, a score of Low was assigned. Although a single LD_{50} of 1,870 mg/kg in rats was identified, this value was an outlier as all other acute oral LD_{50} values range from 5,400-8,000 mg/kg. The weight of evidence indicates that it is not acutely toxic via the oral route. Inhalation LC_{50} values of and > 33.7 mg/L in a standard 4 hour study and ranging from > 26.76 mg/L/7 to 62.48 mg/L/3h support a Low based on inhalation. Dermal LD_{50} values of 4,032 and 6,730 mg/kg also support a Low.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)* (vH, H, M, or L): M**
Propanol was assigned a score of Moderate for systemic toxicity (single dose) based on respiratory tract irritation in inhalation studies of rats and GHS Category 3 classification in Japan. GreenScreen® criteria classify chemicals as a Moderate hazard for systemic toxicity (single dose) when available data indicate that GHS Category 3 classification for respiratory tract irritation is warranted, or the chemical is classified as GHS Category 3 on a GHS country list (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists
    - *Screening:* Japan METI/MOE – GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure – Category 3

Propanol (CAS# 71-23-8)

- NITE 2006
    - Propanol was classified as GHS Category 3 in Japan based on reports of reduced breathing rates indicative of respiratory tract irritation in mice.
- ECHA 2014a
    - *Oral*: In the acute oral toxicity study in male rats that identified an LD_{50} of 5,400 mg/kg, animals (5/dose) were administered a single dose of 2,520, 5,000, 10,000, or 20,000 mg/kg propanol (purity not specified) via gavage and were observed for 14 days. The only clinical signs reported were hyperemia and distention of the stomach and intestines in rats that died. There were no gross pathological lesions in surviving rats.
    - *Inhalation*: In the acute inhalation study in male and female Sprague-Dawley rats that identified an LC_{50} of > 33.8 mg/L/4h, animals (5/sex/dose) were administered 12.9, 24.3, or 33.8 mg/L propanol ($\geq$ 99.8% purity) via whole body inhalation for 4 hours and animals were observed for 14 days. No mortality was observed, but nasal, respiratory tract, and eye irritation were seen. There were no gross pathological changes at necropsy.
    - *Inhalation*: In the acute inhalation study in male and female Sprague-Dawley rats that identified an LC_{50} of > 26.76 mg/L/7h, animals (12/sex) were administered 26.76 mg/L propanol (99.5% purity) via whole body inhalation for 7 hours and were observed for 14 days. There were no deaths or effects on gross pathology.
- EU 2008
    - In rats that were administered 47.05 mg/L propanol via inhalation for 8 hours or 7 hours, irritation of the mucous membranes and increased respiration were seen. At necropsy, edema and hyperemia of the lung were observed.
    - An RD_{50} (50% decrease in respiratory rate) of 31.76 mg/L for respiratory tract irritation was derived in a study of mice (4/group) that were exposed to concentrations ranging from 10.0 mg/L to 70 mg/L for 10 minutes.

- Based on the weight of evidence, a score of Moderate was assigned. GHS classification in Japan is based on respiratory tract effects in mice, and this classification is supported by respiratory tract irritation and lung edema seen in inhalation toxicity studies of rats. GHS criteria state that clinical and histopathological signs (including hyperemia) of respiratory tract irritation in animals can be used as part of the weight of evidence evaluation to classify as GHS Category 3.

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

Propanol was assigned a score of Low for systemic toxicity (repeated dose) based on subchronic oral toxicity studies of propanol and its metabolite propionic acid. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when no adverse effects are seen below the guidance value of 100 mg/kg/day for an oral study (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ECHA 2014a
    - *Inhalation*: In a subchronic inhalation toxicity study according to OECD Guideline 413 in male and female Wistar rats, animals were administered up to 8,000 mg/m^3 (8.0 mg/L[7]). No significant adverse effects were seen at the highest dose. No additional details were provided. ToxServices identified a NOAEC of 8.0 mg/L.
- EU 2008
    - *Oral*: No adverse effects on body weight, food and water consumption, liver weight, or histology were seen in male rats (strain not specified) that were administered 3,000 mg/kg/day isopropanol (purity not specified) through drinking water for 4 months. No additional details were provided. Authors identified a NOAEL of 3,000 mg/kg.
    - *Oral*: In a non-guideline carcinogenicity study in rats (strain not specified), hepatotoxic effects congestion, steatosis, necrosis, fibrosis, cirrhosis and extramedullary and medullary hyperplasia of the hematopoietic bone marrow parenchyma were seen in rats administered 240 mg/kg twice weekly for a lifetime. Authors concluded that propanol is related to liver toxicity and hematotoxicity. The Institute for Health and Consumer Protection of the European Chemicals Bureau concluded that this study is of limited reliability and cannot be used to derive a NOAEL.

Propionic acid (CAS# 79-09-4)

- OECD 2007, ECHA 2014b

Note: OECD notes that numerous repeated dose toxicity studies of propionic acid focused only on point-of contact effects and outcomes varied with consistency of the diet. These studies were not considered in the GreenScreen® assessment.

    - In a subchronic oral toxicity study in male and female beagle dogs, animals (4-8/sex/dose) were administered propionic acid (> 99% purity) at concentrations of 0, 0.3, 1.0, or 3.0% in the diet (reported in OECD 2007 as 0, 196, 660, or 1,848 mg/kg/day for males and 0, 210, 696, or 1,832 mg/kg/day for females) for 100 days. As subset of animals (4/sex/dose) from the control and high doses were maintained on control diets for a 6-week recovery period. OECD reports that the study was conducted similar to OECD Guidelines. There were no treatment-related deaths or clinical signs of toxicity. There were no effects on body weight, organ weight, ophthalmoscopic examination, hematology, clinical chemistry, or urinalysis. Local point-of-contact lesions (diffuse epithelial hyperplasia of the esophageal mucosa)

[7] 8,000 mg/m^3 * 1 m^3/1,000 L = 8.0 mg/L

were seen in the high dose group, but resolved after a 6-week recovery period. Both OECD identified a NOAEL of 1% (660 mg/kg/day for males and 696 mg/kg/day for females) based on changes to the esophagus at the high dose. ECHA reported a NOAEL of 3% (1,848 mg/kg/day for males and 1,832 mg/kg/day for females) for systemic toxicity. OECD identified this study as the definitive study for the repeated dose toxicity endpoint for the SIDS initial assessment profile for propionic acid.

  - In a subchronic oral toxicity study in male and female Sprague-Dawley rats, animals (20/sex/dose) were administered 0, 0.62, 1.25, 2.5, or 5% propionic acid (100% purity) in a pulverized diet for 90 days. A subset of animals (10/sex/control, low, and high dose) was maintained on a control diet for a 42 day recovery period. OECD reports that the study was conducted similar to OECD Guidelines. There was no treatment-related mortality. Body weight was decreased (statistical significance not reported) in males at the high dose. No additional clinical signs of toxicity were seen. There were no effects on ophthalmoscopic examination, hematology, clinical chemistry, urinalysis, or gross pathology. Rats in the high dose displayed point-of-contact effects in the epithelium of the forestomach mucosa, which resolved after a 6-week recovery period. OECD identified a NOAEL of 2.5 % (reported in OECD 2007 as 1,600 mg/kg/day) based on point-of contact effects, while ECHA identified a more conservative NOAEL of 0.62% (400 mg/kg/day[8]) for point-of contact effects based on a dose dependent increase in the incidence and severity of proliferation-acanthosis and retention-hyperkeratosis of the forestomach mucosa. ECHA identified a NOAEL of 5% (3,200 mg/kg/day) for systemic toxicity.

- Based on the weight of evidence, a score of Low was assigned. Only limited data were available for propanol. The REACH dossier reports on a 90-day inhalation toxicity study, but no experimental details were provided and the study could not be located. Therefore this study was not considered in the assessment. One oral toxicity study in rats was reported with few details and was also not weighed heavily in the assessment. The European Chemicals Bureau used the NOAEL of 3,000 mg/kg/day from a 4-month drinking water study in rats in its risk assessment for propanol. In addition, studies of the metabolite propionic acid demonstrate a low order of toxicity, with NOAEL values of 660 mg/kg/day (for local effects) in a 90-day oral study in rats and 400 mg/kg/day (for local effects) in a 100 day oral study in dogs. No evidence of systemic toxicity was seen in these studies.

Neurotoxicity (N)

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

Propanol was assigned a score of Moderate for neurotoxicity (single dose) based on transient narcotic effects in acute inhalation studies in rats. GreenScreen® criteria classify chemicals as a Moderate hazard for neurotoxicity (single dose) when available data indicate that GHS Category 3 classification is warranted (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC – CLP/GHS Hazard Statements (EU H-Statements) H336 May cause drowsiness or dizziness
  - *Authoritative:* EC – Risk Phrases (EU R-Phrases) R67: Vapors may cause drowsiness and dizziness
  - *Screening:* Patty's Toxicology – Boyes Neurotoxicants (Boyes-N) Neurotoxic
  - *Screening:* Japan METI/MOE – GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure – Category 3
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

[8] 1,600 mg/kg/day * 0.62/2.5 = 400 mg/kg/day

Propanol (CAS# 71-23-8)

- NITE 2006
    - Propanol was classified as GHS Category 3 in Japan based on anesthetic actions in inhalation and oral toxicity studies in rats, mice, and rabbits.
- ECHA 2014a
    - *Inhalation*: In the acute inhalation study in male and female rats that identified an LC_{50} of > 33.8 mg/L/4h, animals (5/sex/dose) were administered 12.9, 24.3, or 33.8 mg/L propanol (≥ 99.8% purity) via whole body inhalation for 4 hours and animals were observed for 14 days. Narcosis was observed within 2.5 hours. Symptoms included hypoactivity, prostration, reduced pain reflex, and absence of surface right reflexes. No clinical signs were seen during the 14-day recovery period.
    - *Inhalation*: In the acute inhalation study in male and female Wistar rats that identified LC_{50} values of > 51.91 mg/L/8h and > 62.48 mg/L/3h, animals (6/dose)(were exposed to propanol (99.5% purity) at concentrations of 51.91 mg/L for 8 hours or 62.48 mg/L for 3 hours via whole body inhalation. All animals were in deep anesthesia by the end of exposure and there was a slight decrease in pain reflex. All narcotic effects resolved by 24 hour after exposure.
    - *Inhalation*: In the acute inhalation study in male and female Sprague-Dawley rats that identified an LC_{50} of > 26.76 mg/L/7h, animals (12/sex) were administered 26.76 mg/L propanol (99.5% purity) via whole body inhalation for 7 hours. Accelerated breathing and loss of pain reflex was seen after 3 hours.
- EU 2008
    - *Oral*: A mean acute narcotic dose of 1,441 mg/kg was reported for rabbits. No additional details were provided.
- Based on the weight of evidence, a score of Moderate was assigned. Propanol is associated with the H-Statement H336 May cause drowsiness or dizziness and R-Phrase R67: Vapors may cause drowsiness and dizziness, which correspond to a Low or Moderate. Acute narcotic effects were seen in several acute inhalation studies in rats, which indicates that GHS Category 3 classification is appropriate. This is also consistent with GHS classification in Japan and corresponds to a score of Moderate.

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

Propanol was assigned a score of Data Gap for neurotoxicity (repeated dose) based on a lack of sufficient data for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements) H336 May cause drowsiness or dizziness
    - *Authoritative:* EC - Risk Phrases (EU R-Phrases) R67: Vapors may cause drowsiness and dizziness
    - *Screening:* Patty's Toxicology - Boyes Neurotoxicants (Boyes-N) Neurotoxic
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

Propanol (CAS# 71-23-8)

- EU 2008
    - Neonatal rats (number and strain not specified) that were exposed to propanol (purity not specified) at doses of 3,000, 3,800, 7,500, or 7,800 mg/kg via intubation on postnatal days 5, 6, 7, and 8 showed signs of intoxication including impaired righting response. Effects were considered to be a result of acute intoxication as there was no indication of dose dependency.

Propionic acid (CAS# 79-09-4)

- No data were identified

- Based on the weight of evidence, a data gap was assigned. No subchronic or chronic studies were identified for propanol or its metabolite in order to determine if repeated propanol exposure results in neurotoxicity.

Skin Sensitization (SnS) Group II* Score (H, M, or L): L
Propanol was assigned a score of Low for skin sensitization based on negative results in a guinea pig maximization test, mouse ear swelling test, and human patch test. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and are negative for sensitization, and the chemical is not present on authoritative or screening lists (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ECHA 2014a
  - Propanol was negative in a guinea pig maximization test similar to OECD Guideline 406 (no pretreatment of skin with SDS before topical induction, time of evaluation after challenge not stated) in Hartley guinea pigs (15/test, 6/control, sex not specified) that were induced topically and subcutaneously with 100% propanol (> 99.8% purity) and challenged with a 100% solution. No positive reactions were seen in any animal upon challenge.
  - Propanol was negative in a mouse ear swelling test in female CF-1 mice. Animals (10/treatment, 5/control) were induced topically and subcutaneously with 100% propanol (98% purity) and were challenged 7 days after induction with 100% propanol. No positive reactions were seen in any animal upon challenge.
- NICNAS 2013
  - There has been one case report of a laboratory worker testing in a patch test of propanol. There were no positive reactions in a patch test of 50 human volunteers that were induced with a total of 9 24-hour applications of 0.2 mL propanol during the course of 3 weeks followed by challenge 10-14 days later.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG
Propanol was assigned a score of Data Gap for respiratory sensitization based on a lack of data for this endpoint.

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

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): L
Propanol was assigned a score of Low for skin irritation/corrosivity based on negative results in dermal irritation studies in rabbits. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and indicate that the chemical does not warrant GHS classification (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists
  - *Screening:* Japan METI/MOE - GHS Classifications (GHS-Japan) Skin corrosion / irritation - Category 2

Propanol (CAS# 71-23-8)

- NITE 2006
  - Propanol is classified as GHS Category 2 in Japan based on a report of erythema in 9/12 humans.
- ESIS 2000
  - Propanol is reported as causing no irritation to moderate irritation in rabbits, and was classified as not irritating by EC criteria. No additional details were provided.
  - Propanol was not irritating in a patch test in humans. No additional details were available (report in German).
- ECHA 2014a
  - Propanol (99.5% purity) was not irritating in a dermal irritation test similar to OECD Guideline 404 in 2 male Vienna White rabbits that were administered 1 mL to shaved skin for 1, 5, or 15 minutes, or 20 hours under occlusion. Following the 20 hour exposure, the mean scores at 24, 48, and 72 hours were 0.33/4 for erythema and 0/4 for edema. Flaky skin was observed in 1 animal after 20 hours of exposure. Authors concluded that the substance is not irritating.
  - Propanol (purity not specified) was not irritating when 0.5 mL was administered to the intact or abraded skin of male albino rabbits (3/intact, 3/abraded) on square gauze patches for 24 hours. The primary irritation score for all animals was 0.
  - Propanol (100% purity assumed) was not irritating in a dermal irritation test similar to OECD Guideline 404 in 2 male Vienna White rabbits that were administered 1 mL to shaved skin for 1, 5, or 15 minutes, or 20 hours under occlusion. Following the 20 hour exposure, the mean scores at 24, 48, and 72 hours were 0 for both erythema and edema. Authors concluded that the substance is not irritating.
- NICNAS 2013
  - Erythema was seen in 7/10 human volunteers in a patch test that was conducted immediately after the forearm was immersed in 33 °C water for 10 minutes. No erythema was seen on forearms that were not hydrated prior to testing.
- Based on the weight of evidence, a score of Low was assigned. Japan's GHS classification is based on a report erythema in a human patch test, but no details were provided and the study could not be located. All available animal data and a human patch test demonstrating a lack of effects on skin that was not pre-hydrated indicate that this chemical does not warrant GHS classification for skin irritation. Therefore a score of Low was assigned.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): vH

Propanol was assigned a score of Very High for eye irritation/corrosivity based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a Very High hazard for eye irritation/corrosivity when the chemical is associated with the H-Statement H318 Causes serious eye damage and R-Phrase R41: Risk of serious damage to eyes (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EC - CLP/GHS Hazard Statements (EU H-Statements) H318 Causes serious eye damage
  - *Authoritative:* EC - Risk Phrases (EU R-Phrases) R41: Risk of serious damage to eyes
  - *Screening:* New Zealand HSNO/GHS (GHS-New Zealand) 6.4A - Irritating to the eye (Category 2A)
  - *Screening*: Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2A.

Ecotoxicity (Ecotox)

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

Propanol was assigned a score of Low for acute aquatic toxicity based on an LC_{50} of 3,800 mg/L in fish, EC_{50} of 1,000 mg/L in daphnia, and EC_{03} of 3,100 mg/L in algae. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when the most conservative LC/EC_{50} values are greater than 100 mg/L, and the chemical is not present on authoritative or screening lists (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ECHA 2014a
  - 96-hour LC_{50} (*Pimephales promelas*, fathead minnow) = 4,555 mg/L
  - 96-hour LC_{50} (*Alburnus alburnus*, bleak) = 3,800 mg/L
  - 96-hour LC_{50} (*Pimephales promelas*, fathead minnow) = 4,650 mg/L
  - 48-hour EC_{50} (*Gammarus pulex*, freshwater amphipod) = 1,000 mg/L
  - 48-hour EC_{50} (*Daphnia magna*, water flea) = 3,644 mg/L
  - 48-hour EC_{50} (*Pseudokirchneriella subcapitata*, green algae) = 9,170 mg/L (growth)
  - 48-hour EC_{50} (*Chlorella pyrenoidosa*, green algae) > 1,150 mg/L (growth)
  - 48-hour EC_{50} (*Selenastrum capricornutum*, green algae) > 2,000 mg/L (growth)
  - 48-hour EC_{50} (*Scenedesmus pannonicus*, green algae) > 2,900 mg/L (growth)
  - 192-hour EC_{03} (*Scenedesmus quadricauda*, green algae) = 3,100 mg/L
- Based on the weight of evidence, a score of Low was assigned. No standard-length acute studies were available for algae, but the 192-hour EC03 of 3,100 mg/L indicates that the 72-hour EC_{50} is > 100 mg/L.

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

Propanol was assigned a score of Low for chronic aquatic toxicity based on a measured 21-day NOEC of greater than 100 mg/L in daphnia and modeled ChV of 148.7 mg/L in fish and 62.1 mg/L in algae. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when chronic aquatic toxicity values are greater than 10 mg/L (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ECHA 2014a
  - 21-day NOEC (*Daphnia magna*, water flea) > 100 mg/L (reproduction)
- U.S. EPA 2012a
  - Propanol is designated to the Neutral Organics ECOSAR chemical class. The most conservative predicted ChV values are 148.7 mg/L in fish, 55.3 mg/L in daphnia, and 62.1 mg/L in green algae.
- Based on the weight of evidence, a score of Low was assigned. Measured data were available only for daphnia, but acute toxicity studies do not indicate that fish and plants are more sensitive than invertebrates. Modeled data for all three trophic levels also support a score of Low.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): vL
Propanol was assigned a score of Very Low for persistence based on being readily biodegradable in two biodegradation assays. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence when the chemical partitions primarily to soil and water, and the chemical meets the 10-day biodegradation window (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ECHA 2014a
  - In a ready biodegradation assay (BOD-Standard Methods for the Examination of Water and Wastewater. 1971. 13th Ed. American Public Health Association, New York, NY) using domestic non-adapted sewage inoculum, propanol (3 mg/L) achieved 64% biodegradation in 5 days, 76% in 10 days, 81% in 15 days, and 75% in 20 days. Authors concluded that the substance is readily biodegradable.
  - In a ready biodegradation test according to OECD Guideline 301D (Ready Biodegradability: Closed Bottle Test) using domestic non-adapted sewage inoculum, propanol (starting concentration not reported) achieved 71% biodegradation in 5 days and 81% biodegradation in 15 days. Authors concluded that the substance is readily biodegradable.
- U.S. EPA 2012b
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that propanol is not expected to be readily biodegradable. Fugacity modeling predicts 50.7% will partition to soil with a half-life of 30 days, 44.9% will partition to water with a half-life of 15 days, and 4.29% will partition to air with a half-life of 46.4 hours.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
Propanol was assigned a score of Very Low for bioaccumulation based on a measured log K_{ow} of 0.25. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when the log K_{ow} is less than 4 (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- ChemIDplus 2014
  - Propanol has an experimental log K_{ow} of 0.25.
- U.S. EPA 2012b
  - BCFBAF predicts a BCF of 1.011 based on a log K_{ow} of 0.25, indicating this chemical is not likely to bioaccumulate because the BCF is less than 100 based on a log K_{ow} less than 5.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Propanol was assigned a score of Low for reactivity based on not being explosive or oxidizing based on structural properties. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when the chemical has no explosive or oxidizing properties, and the chemical is not present on authoritative or screening lists (CPA 2012a).

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

Propanol (CAS# 71-23-8)

- EU 2008
    - Propanol is not explosive based on structural properties.
    - Propanol is not oxidizing based on structural properties.

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

Propanol was assigned a score of High for flammability based on presence on authoritative lists. GreenScreen® criteria classify chemicals as a High hazard for flammability when the chemical is classified as U.S. DOT Hazard Class 3 Packing Group II and is associated with the H-Statement H225 Highly flammable liquid and vapor (CPA 2012a).

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

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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 Propanol (CAS #71-23-8)

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	**Propanol**	**71-23-8**	*L*	**L**	*M*	**M**	DG	**L**	**M**	**L**	**M**	DG	**L**	DG	**L**	**vH**	**L**	**L**	**vL**	**vL**	*L*	**H**

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	Yes	Yes
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Propanol	2

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

Table 6

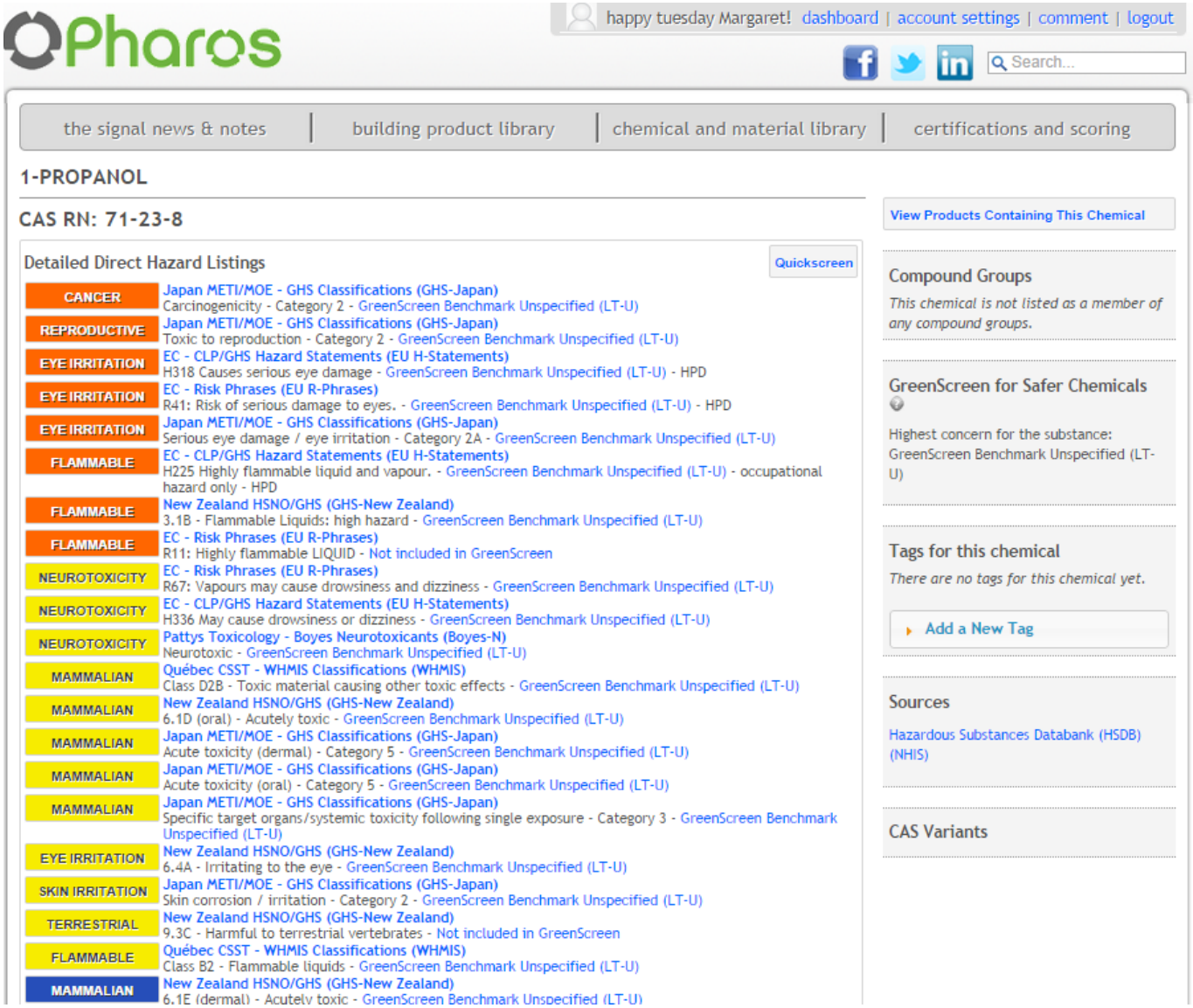
Chemical Name	Final GreenScreen® Benchmark Score
Propanol	2

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 Propanol (CAS #71-23-8)



Pharos

happy tuesday Margaret! dashboard | account settings | comment | logout

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1-PROPANOL

CAS RN: 71-23-8

Detailed Direct Hazard Listings — Quickscreen

CANCER	Japan METI/MOE - GHS Classifications (GHS-Japan) Carcinogenicity - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
REPRODUCTIVE	Japan METI/MOE - GHS Classifications (GHS-Japan) Toxic to reproduction - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
EYE IRRITATION	EC - CLP/GHS Hazard Statements (EU H-Statements) H318 Causes serious eye damage - GreenScreen Benchmark Unspecified (LT-U) - HPD
EYE IRRITATION	EC - Risk Phrases (EU R-Phrases) R41: Risk of serious damage to eyes. - GreenScreen Benchmark Unspecified (LT-U) - HPD
EYE IRRITATION	Japan METI/MOE - GHS Classifications (GHS-Japan) Serious eye damage / eye irritation - Category 2A - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	EC - CLP/GHS Hazard Statements (EU H-Statements) H225 Highly flammable liquid and vapour. - GreenScreen Benchmark Unspecified (LT-U) - occupational hazard only - HPD
FLAMMABLE	New Zealand HSNO/GHS (GHS-New Zealand) 3.1B - Flammable Liquids: high hazard - GreenScreen Benchmark Unspecified (LT-U)
FLAMMABLE	EC - Risk Phrases (EU R-Phrases) R11: Highly flammable LIQUID - Not included in GreenScreen
NEUROTOXICITY	EC - Risk Phrases (EU R-Phrases) R67: Vapours may cause drowsiness and dizziness - GreenScreen Benchmark Unspecified (LT-U)
NEUROTOXICITY	EC - CLP/GHS Hazard Statements (EU H-Statements) H336 May cause drowsiness or dizziness - GreenScreen Benchmark Unspecified (LT-U)
NEUROTOXICITY	Pattys Toxicology - Boyes Neurotoxicants (Boyes-N) Neurotoxic - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Québec CSST - WHMIS Classifications (WHMIS) Class D2B - Toxic material causing other toxic effects - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	New Zealand HSNO/GHS (GHS-New Zealand) 6.1D (oral) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (dermal) - Category 5 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) Acute toxicity (oral) - Category 5 - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	Japan METI/MOE - GHS Classifications (GHS-Japan) Specific target organs/systemic toxicity following single exposure - Category 3 - GreenScreen Benchmark Unspecified (LT-U)
EYE IRRITATION	New Zealand HSNO/GHS (GHS-New Zealand) 6.4A - Irritating to the eye - GreenScreen Benchmark Unspecified (LT-U)
SKIN IRRITATION	Japan METI/MOE - GHS Classifications (GHS-Japan) Skin corrosion / irritation - Category 2 - GreenScreen Benchmark Unspecified (LT-U)
TERRESTRIAL	New Zealand HSNO/GHS (GHS-New Zealand) 9.3C - Harmful to terrestrial vertebrates - Not included in GreenScreen
FLAMMABLE	Québec CSST - WHMIS Classifications (WHMIS) Class B2 - Flammable liquids - GreenScreen Benchmark Unspecified (LT-U)
MAMMALIAN	New Zealand HSNO/GHS (GHS-New Zealand) 6.1E (dermal) - Acutely toxic - GreenScreen Benchmark Unspecified (LT-U)

View Products Containing This Chemical

Compound Groups

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

GreenScreen for Safer Chemicals

Highest concern for the substance: GreenScreen Benchmark Unspecified (LT-U)

Tags for this chemical

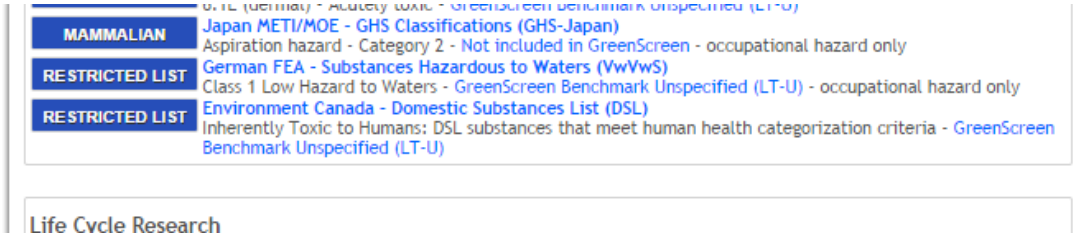
There are no tags for this chemical yet.

Add a New Tag

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants



APPENDIX D: ECOSAR Modeling Results for Propanol (CAS #71-23-8)

ECOSAR Version 1.11 Results Page

SMILES: OCCC
CHEM: 1-Propanol
CAS Num: 000071-23-8
ChemID1:
MOL FOR: C3 H8 O1
MOL WT: 60.10
Log K_{ow}: 0.350 (EPISuite K_{ow}win v1.68 Estimate)
Log K_{ow}: 0.250 (User Entered)
Log K_{ow}: 0.25 (PhysProp DB exp value - for comparison only)
Melt Pt: -126.00 (deg C, User Entered for Wat Sol estimate)
Melt Pt: -126.10 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 2.932E+005 (mg/L, EPISuite WSK_{ow}win v1.43 Estimate)
Wat Sol: 1E+006 (mg/L, User Entered)
Wat Sol: 1E+006 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log K_{ow}: 0.250 (User Entered)
Wat Sol: 1E+006 (mg/L, User Entered)

Available Measured Data from ECOSAR Training Set

CAS No	Organism	Duration	End Pt	Measured mg/L (ppm)	Ecosar Class	Reference
000071-23-8	Daphnid	48-hr	LC50	3644	Neutral organics	Kuhn, 1989
000071-23-8	Fish	96-hr	LC50	4480	Neutral organics	DUL
000071-23-8	Fish	96-hr	LC50	4630	Neutral organics	DUL

ECOSAR v1.1 Class-specific Estimations

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	1841.305

Neutral Organics	: Daphnid	48-hr	LC50	889.509
Neutral Organics	: Green Algae	96-hr	EC50	339.704
Neutral Organics	: Fish		ChV	148.748
Neutral Organics	: Daphnid		ChV	55.329
Neutral Organics	: Green Algae		ChV	62.076
Neutral Organics	: Fish (SW)	96-hr	LC50	2293.906
Neutral Organics	: Mysid	96-hr	LC50	5578.605
Neutral Organics	: Fish (SW)		ChV	85.522
Neutral Organics	: Mysid (SW)		ChV	809.936
Neutral Organics	: Earthworm	14-day	LC50	158.681

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

Class Specific LogK_{ow} Cut-Offs

If the log K_{ow} of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogK_{ow}: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogK_{ow}: 6.0 (Earthworm LC50)
Maximum LogK_{ow}: 6.4 (Green Algae EC50)
Maximum LogK_{ow}: 8.0 (ChV)

APPENDIX E: EPISuite Modeling Results for Propanol (CAS #71-23-8)

CAS Number: 71-23-8
SMILES: OCCC
CHEM: 1-Propanol
MOL FOR: C3 H8 O1
MOL WT: 60.10
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log K_{ow} (octanol-water): 0.25
Boiling Point (deg C): 97.20
Melting Point (deg C): -126.00
Vapor Pressure (mm Hg): 21
Water Solubility (mg/L): 1E+006
Henry LC (atm-m^3/mole): 7.41E-006

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (K_{ow}WIN v1.68 estimate) = 0.35
Log K_{ow} (Exper. database match) = 0.25
Exper. Ref: HANSCH, C. ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 89.96 (Adapted Stein & Brown method)
Melting Pt (deg C): -74.95 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 23.2 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C): 3.09E+003 (Mean VP of Antoine & Grain methods)
MP (exp database): -126.1 deg C
BP (exp database): 97.2 deg C
VP (exp database): 2.10E+01 mm Hg (2.80E+003 Pa) at 25 deg C

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 2.932e+005
log K_{ow} used: 0.25 (user entered)
melt pt used: -126.00 deg C
Water Sol (Exper. database match) = 1e+006 mg/L (25 deg C)
Exper. Ref: RIDDICK, J.A. ET AL. (1986)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1.714e+005 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 7.52E-006 atm-m^3/mole (7.62E-001 Pa-m^3/mole)
Group Method: 6.89E-006 atm-m^3/mole (6.99E-001 Pa-m^3/mole)
Exper Database: 7.41E-06 atm-m^3/mole (7.51E-001 Pa-m^3/mole)
For Henry LC Comparison Purposes:

User-Entered Henry LC: 7.410E-006 atm-m^3/mole (7.508E-001 Pa-m^3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.661E-006 atm-m^3/mole (1.683E-001 Pa-m^3/mole)
VP: 21 mm Hg (source: User-Entered)
WS: 1E+006 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 0.25 (user entered)
Log K_{aw} used: -3.519 (user entered)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 3.769
Log K_{oa} (experimental database): 3.710

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.8777
Biowin2 (Non-Linear Model): 0.9635
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.2263 (weeks)
Biowin4 (Primary Survey Model): 3.8905 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.7937
Biowin6 (MITI Non-Linear Model): 0.9354
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.9413
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): 2.8E+003 Pa (21 mm Hg)
Log K_{oa} (Exp database): 3.710
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model: 1.07E-009
Octanol/air (K_{oa}) model: 1.26E-009
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 3.87E-008
Mackay model: 8.57E-008
Octanol/air (K_{oa}) model: 1.01E-007

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 5.4770 E-12 cm^3/molecule-sec
Half-Life = 1.953 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 23.435 Hrs.
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
6.22E-008 (Junge-Pankow, Mackay avg)
1.01E-007 (K_{oa} method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
K_{oc}: 1.904 L/kg (MCI method)
Log K_{oc}: 0.280 (MCI method)
K_{oc}: 4.487 L/kg (K_{ow} method)
Log K_{oc}: 0.652 (K_{ow} method)
Experimental Log K_{oc}: 0.48 (database)

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

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.3824 days (HL = 0.04146 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.005 (BCF = 1.011)
Log BAF Arnot-Gobas method (upper trophic) = 0.005 (BAF = 1.011)
log K_{ow} used: 0.25 (user entered)

Volatilization from Water:
Henry LC: 7.41E-006 atm-m^3/mole (entered by user)
Half-Life from Model River: 62.04 hours (2.585 days)
Half-Life from Model Lake: 741.9 hours (30.91 days)

Removal in Wastewater Treatment:
Total removal: 92.07 percent
Total biodegradation: 91.67 percent
Total sludge adsorption: 0.34 percent
Total to Air: 0.07 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	4.29	46.4	1000
Water	44.9	360	1000
Soil	50.7	720	1000
Sediment	0.0857	3.24e+003	0

Persistence Time: 348 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

Propanol GreenScreen® Evaluation Prepared by:

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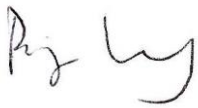
Propanol GreenScreen® Evaluation QC'd by:



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