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PENTYLENE GLYCOL

(CAS #5343-92-0)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: March 18, 2024

Expiration Date: March 18, 2029

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TABLE OF CONTENTS

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Content Copyright © (2024) by ToxServices. All rights reserved.

TABLE OF FIGURES

TABLE OF TABLES

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GreenScreen® Executive Summary for Pentylene Glycol (CAS #5343-92-0)

Pentylene glycol is a non-flammable colorless to slightly yellow liquid at standard temperature and pressure. It is a short chain 1,2-glycol commonly used as a skin and hair conditioning agent and viscosity controlling agent in personal care products. It is also used as a solvent in cosmetics, cleaning products, polishes and wax blends, inks and toners, and fragrances. It is produced via catalytic oxidation of the corresponding alkene oxide or reduction of the corresponding 2-hydroxy acid.

Pentylene glycol was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes"). This score is based on the following hazard score:

- Benchmark 2f
    - Very High Group II Human Toxicity (eye irritation-IrE)

A data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), pentylene glycol meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if pentylene glycol were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

New Approach Methodologies (NAMs) used in this GreenScreen® include *in silico* modeling for carcinogenicity, endocrine activity, respiratory sensitization, aquatic toxicity, persistence, and bioaccumulation, and *in vitro* testing for mutagenicity. The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties:

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

Type I (input data) uncertainties in pentylene glycol's NAMs dataset include lack of/insufficient experimental data for carcinogenicity, endocrine activity, respiratory sensitization, and chronic aquatic toxicity, and lack of validated test methods for respiratory sensitization. Pentylene glycol's Type II (extrapolation output) uncertainties include the lack of defined applicability domains in some modeling programs, limitation of *in vitro* genotoxicity assays in mimicking *in vivo* metabolism, their focusing on one or only a few types of genotoxicity events, the uncertain *in vivo* relevance of *in silico* modeling of receptor reactivity due to lack of consideration of toxicokinetics, and the limitation of OECD Toolbox in identifying structural alerts for respiratory sensitization without accounting for non-immunologic mechanisms of respiratory sensitization.

GreenScreen® Hazard Summary Table for Pentylene Glycol

Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	*L*	**L**	DG	**L**	**L**	**L**	*M*	**L**	**L**	*L*	**L**	**vH**	**L**	*L*	*M*	**vL**	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. 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. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

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GreenScreen® Chemical Assessment for Pentylene Glycol (CAS #5343-92-0)

Method Version: GreenScreen® Version 1.4
Assessment Type[1]: Certified
Assessor Type: Licensed GreenScreen® Profiler

GreenScreen® Assessment (v.1.4) Prepared By:
Name: Rachel Doerer, M.P.H.
Title: Toxicologist
Organization: ToxServices LLC
Date: January 16, 2024; March 11, 2024

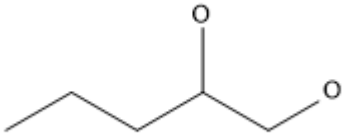
Quality Control Performed By:
Name: Bingxuan Wang, Ph.D., D.A.B.T.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: February 22, 2024; March 18, 2024

Expiration Date: March 18, 2029[2]

Chemical Name: Pentylene glycol

CAS Number: 5343-92-0

Chemical Structure(s):



Also called:
1,2-Pentanediol; Pentane-1,2-diol; 1,2-Dihydroxypentane (PubChem 2024)

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Pentylene glycol has a relatively complete toxicological dataset; however, data gaps exist for carcinogenicity, reproductive toxicity, and developmental toxicity. For these endpoints, data on the structurally related short chain 1,2-glycols 1,2-butanediol (CAS #584-03-2) and 1,2-hexanediol (CAS #6920-22-5) were considered. These surrogates differ from the target chemical only in the length of the carbon backbone attached to the hydroxyl groups at the 1 and 2 positions, with 1,2-butanediol having 1 less carbon than pentylene glycol and 1,2-hexanediol having 1 more carbon than pentylene glycol. Due to their close stuructural similarity, they are expected to be strong surrogates. Additionally, these chemicals were used in the ECHA REACH dossier for pentylene glycol as key read across chemicals (ECHA, CAS #5343-92-0, 2024). No data were identified for the target substance or its surrogates for the carcinogenicty endpoint, therefore, ToxServices used a shorter 1,2-glycol, propylene glycol (CAS #57-55-6) as a conservative surrogate and performed modeling to evaluate this endpoint. Propylene glycol is 2 carbons shorter than the pentylene glycol.

[1] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), or "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent).
[2] Assessments expire five years from the date of completion starting from January 1, 2019. An assessment expires three years from the date of completion if completed before January 1, 2019 (CPA 2018a).

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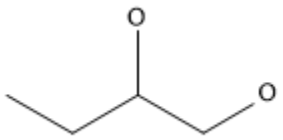
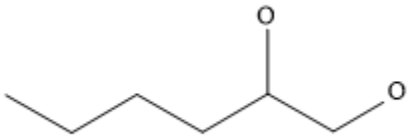
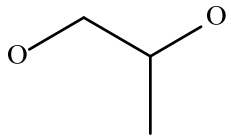


1,2-Butanediol (CAS #584-03-2)



1,2-Hexanediol (CAS #6920-22-5)



Propylene glycol (CAS #57-55-6)

Identify Applications/Functional Uses: (EC 2024, U.S. EPA 2023, CIR 2012)
1. Skin conditioning agent
2. Solvent
3. Hair conditioning agent
4. Viscosity increasing agent

Known Impurities[3]:
No information is available. The screen is performed on the theoretical pure substance.

GreenScreen® Summary Rating for Pentylene Glycol[4,5 6,7]: Pentylene glycol was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes") (CPA 2018b). This score is based on the following hazard score:

- Benchmark 2f
    - Very High Group II Human Toxicity (eye irritation-IrE)

A Data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), pentylene glycol meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if

[3] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.
[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] See Appendix A for a glossary of hazard endpoint acronyms.
[6] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[7] For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen® Guidance v1.4 Annex 2.

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pentylene glycol were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary Table for Pentylene Glycol

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	*L*	**L**	DG	**L**	**L**	**L**	*M*	**L**	**L**	*L*	**L**	**vH**	**L**	*L*	*M*	**vL**	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. 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. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

Environmental Transformation Products

No transformation products were identified for pentylene glycol. Due to the lack of functional groups that are hydrolytically reactive, hydrolysis is not expected and will not significantly contribute to the removal of pentylene glycol from the environment (ECHA, CAS #5343-92-0, 2024).

Introduction

Pentylene glycol is a short chain 1,2-glycol. It is produced via catalytic oxidation of the corresponding alkene oxide or reduction of the corresponding 2-hydroxy acid (CIR 2012).

ToxServices assessed pentylene glycol against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2021).

U.S. EPA Safer Choice Program's Safer Chemical Ingredients List

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2023). It can be accessed at: http://www2.epa.gov/saferchoice/safer-ingredients. Chemicals on the SCIL have been assessed for compliance with the Safer Choice Standard and Criteria for Safer Chemical Ingredients (U.S. EPA 2015).

Pentylene glycol is listed on the U.S. EPA SCIL as a solvent with a Full Green Circle.

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 2018b). Pharos (Pharos 2024) is an online list-searching tool that is used to screen chemicals against all of the lists in the List Translator electronically. ToxServices also checks the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b),[8] which are not considered GreenScreen® Specified Lists but are additional information sources, in conjunction with the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for pentylene glycol can be found in Appendix C.

[8] DOT lists are not required lists for GreenScreen® List Translator v1.4. They are reference lists only.

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- Pentylene glycol is an LT-UNK chemical when screened using Pharos, and therefore a full GreenScreen® is required.
- Pentylene glycol is not listed on the U.S. DOT list.
- Pentylene glycol is on the following list for multiple endpoints. Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.
    - German FEA – Substances Hazardous to Waters – Class 1 – Low Hazard to Waters

Hazard Statement and Occupational Control

No Globally Harmonized System of Classification and Labelling of Chemicals (GHS) hazard statements (H-Statements) that were harmonized across the European Union (EU) were identified for pentylene glycol. H-Statements reported in the ECHA REACH dossier are reported in Table 1. General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OELs) were identified.

Table 1: GHS H Statements for Pentylene Glycol (CAS #5343-92-0) (ECHA, CAS #5343-92-0, 2024)

H Statement	H Statement Details
H318	Causes serious eye damage

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Pentylene Glycol (CAS #5343-92-0)

Personal Protective Equipment (PPE)	Reference	Occupational Exposure Limits (OEL)	Reference
Safety glasses with side shields or goggles; protective gloves and clothing; respiratory protection when exposure limits are exceeded	Santa Cruz Biotechnology 2022	None identified	N/A

Physicochemical Properties of Pentylene Glycol

Pentylene glycol is a colorless to slightly yellow liquid at standard temperature and pressure. It is slightly volatile and completely miscible in water. Its log K_{ow} of 0.06 indicates it is not likely to bioaccumulate.

Table 3: Physical and Chemical Properties of Pentylene Glycol (CAS #5343-92-0)

Property	Value	Reference
Molecular formula	$C_5H_{12}O_2$	PubChem 2024
SMILES Notation	CCCC(CO)O	PubChem 2024
Molecular weight	104.15 g/mol	PubChem 2024
Physical state	Liquid	ECHA, CAS #5343-92-0, 2024
Appearance	Colorless to slightly yellow	ECHA, CAS #5343-92-0, 2024
Melting point	-40°C	ECHA, CAS #5343-92-0, 2024
Boiling point	209.4°C	ECHA, CAS #5343-92-0, 2024
Vapor pressure	0.015 hPa (0.011 mm Hg) at 20°C	ECHA, CAS #5343-92-0, 2024

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Table 3: Physical and Chemical Properties of Pentylene Glycol (CAS #5343-92-0)		
Property	**Value**	**Reference**
Water solubility	1,000 g/L at 20°C	ECHA, CAS #5343-92-0, 2024
Dissociation constant	Not applicable	
Density/specific gravity	0.98 g/cm^3 at 20°C	ECHA, CAS #5343-92-0, 2024
Partition coefficient	Log K_{ow} = 0.06 at 25°C	ECHA, CAS #5343-92-0, 2024

Toxicokinetics

No experimental toxicokinetic data are identified for pentylene glycol, specifically.

When a 1 g/kg dose of the surrogate 1,2-butanediol was intravenously infused into rabbits, metabolism was described as slow, it was excreted in the urine either unchanged or as the glucuronide, and there was no accumulation in tissues (CIR 2012).

Pentylene glycol is estimated to be excreted in the urine unchanged or conjugated to glucoronidate or sulphate. As there is no clear hint for a first pass effect in the liver, a significant amount may be excreted unchanged (ECHA, CAS #5343-92-0, 2024).

Due to high water solubility and possible metabolism pentylene glycol is unlikely to accumulate in the body (ECHA, CAS #5343-92-0, 2024).

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

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

Pentylene glycol was assigned a score of Low for carcinogenicity based on negative experimental data for the surrogate propylene glycol, and on the weight of evidence from rule-based (VEGA, Toxtree, and OncoLogic) and statistical-based (Danish QSAR) modeling programs. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is high based on reliable data on a conservative surrogate supported by modeled data on the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- UNEP 2001, ECHA, CAS #57-55-6, 2024, CIR 2012
  - *Oral: Surrogate: Propylene glycol (CAS #57-55-6):* A non-GLP compliant 2-year chronic toxicity/carcinogenicity study (guideline not reported) was conducted using male and female Crj: CD(SD) rats (30/sex/dose group). Rats were provided diets containing propylene glycol (purity not specified) at 0, 6,250, 12,500, 25,000, or 50,000 ppm (reported to be equivalent to 0, 200, 400, 900, and 1,700 mg/kg/day for males and 0, 300, 500, 1,000, and 2,100 mg/kg/day for females, respectively) for 2 years. No evidence of treatment-related tumor induction was observed with treatment (Klimisch 2, reliable with restrictions) (Gaunt et al. 1972).

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- *Oral:* *Surrogate: Propylene glycol (CAS #57-55-6):* A non-GLP compliant 2-year chronic toxicity/carcinogenicity study (guideline not reported) was conducted using male and female rats (strain not specified). Animals were exposed via drinking water at 0, 1, 2, 5, 10, 25, and 50% (reported to be equivalent to 0, 1,600, 3,680, 7,700, 13,200, 21,000, and 37,000 mg/kg/day) for 140 days (5/sex/dose). Animals were evaluated based on food and water consumption, body weights, urinalysis, gross pathology, and histopathology of the kidneys, heart, spleen, and liver. All animals exposed at ≥ 25% died within the first 9 days of exposure. Food intake was slightly reduced in the 10% group compared to controls; however, there were no significant effects on water consumption or body weights in groups exposed at up to 10%. Albuminuria, cells, or casts in the urine were identified in animals administered 1 to 10% solutions (no further details provided). There were no significant findings based on gross pathology or histopathology in rats exposed at up to 10%. The NOAEL was assigned at 13,200 mg/kg/day (Klimisch 2, reliable with restrictions) (Seidenfeld and Hanzlik 1932).
- *Oral:* *Surrogate: Propylene glycol (CAS #57-55-6):* Albino rats were provided diets containing propylene glycol (purity not specified) at 0, 2.45 and 4.9% in the diet for 2 years (6 males and 4 females/dose). Animals were evaluated based on cage side observations, food and water consumption, body weights, food efficiency, gross pathology, and histopathology of the lung, heart, liver, kidney, adrenal, and testis (routinely), and the pancreas, stomach, intestines, and lymph in about half of the animals, and other organs occasionally. Slight chronic liver damage was the only effect reported (no further details provided). The NOAEL was assigned at 4.9% in the diet (Klimisch 2, reliable with restrictions) (Morris et al. 1941).
- *Oral:* *Surrogate: Propylene glycol (CAS #57-55-6):* A non-GLP compliant 2-year chronic toxicity/carcinogenicity study (method not reported) was conducted using male and female Beagle dogs (5/sex/dose group). Dogs were provided food containing propylene glycol (USP) at 0, 8%, or 20% (equivalent to 0, 2,000, and 5,000 mg/kg/day, respectively) for 2 years. Tumor incidences were unchanged in male and female dogs when compared to the controls (Klimisch 2, reliable with restrictions) (Weil et al. 1971).
- *Dermal:* *Surrogate: Propylene glycol (CAS #57-55-6):* In a skin painting study, propylene glycol was administered to female mice at 2, 10 or 21 mg/day over the lifetime. No increase in dermal tumors was observed (Klimisch 2, reliable with restrictions) (Stenbäck and Shubik 1974).
- *Inhalation:* *Surrogate: Propylene glycol (CAS #57-55-6):* Groups of 20 white rats were exposed to a supersaturated atmosphere with propylene glycol vapor (> 350 mg/m^3), whole-body, 24 hours/day, for up to 18 months. The number of rats was increased by birth of young. Observations in life were recorded for body weight gain, coat color, conjunctival effects, number of young born, and general conditions. Rats were sacrificed at intervals of 3 to 18 months from the beginning of exposure. Urine was aspirated from the bladder for urinalysis, gross pathological and histopathological (lungs, liver, kidney, and spleen) examinations were performed. There were no increases in tumor incidence observed (Klimisch 2, reliable with restrictions) (Robertson et al. 1947).
- *Inhalation:* *Surrogate: Propylene glycol (CAS #57-55-6):* Two groups of Macaca Rhesus monkeys were exposed to propylene glycol vapor at 100 to 220 mg/m^3 (about 60% saturation), and > 350 mg/m^3 (supersaturation), whole-body, 24 hours/day, for 1 to 13 months (14-15 animals/sex/ group, and 16/sex in the control group). Animals were evaluated based on body weight changes, texture and color of hair and skin, condition of eyes, appetite, activity, and any abnormal signs or symptoms. Complete blood counts were performed at the beginning of the experiment, and again just prior to sacrifice. Tests for the

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ability of the kidneys to concentrate urine were conducted at the end of the observation period. Gross pathology and microscopic examinations of the liver, kidneys, spleen, mesenteric glands, adrenals and in certain cases stomach, intestines and tested were performed. Infections with parasitic nematodes and lung mites were found in almost all of the animals. There were no increases in tumor incidence observed (Klimisch 2, reliable with restrictions) (Robertson et al. 1947).

- VEGA 2023
  - ToxServices predicted the carcinogenicity potential of pentylene glycol using the following six VEGA v1.2.3 models: CAESAR v2.1.10, ISS v.1.0.3, IRFMN/ISSCAN-CGX v1.0.2, IRFMN/Antares v1.0.2, IRFMN oral classification v1.0.1, and IRFMN inhalation classification v1.0.1. If an external compound is beyond the defined scope of a given model, it is considered outside that model's applicability domain (AD) and cannot be associated with a reliable prediction (Sahigara 2007). Values for AD index (ADI) range from 0 (worst case) to 1 (best case). Generally, ADI values of > 0.70 indicate that the prediction has moderate or better predictivity (Gad 2016).
    - CAESAR v2.1.10 model predicts pentylene glycol to be a carcinogen with low confidence. The ADI is 0, indicating that the prediction is not reliable (Appendix D).
    - ISS v1.0.3 model predicts pentylene glycol to be a non-carcinogen with low confidence. The ADI is 0.642, indicating that the prediction is not reliable (Appendix D).
    - IRFMN/ISSCAN-CGX v1.0.2 model predicts pentylene glycol to be a possible non-carcinogen with moderate confidence. The ADI is 0.621, indicating that the prediction is not reliable (Appendix D).
    - IRFMN/Antares v1.0.2 model predicts pentylene glycol to be a possible **non-carcinogen** with high confidence. The ADI is **0.838**, indicating that the prediction is reliable (Appendix D).
    - IRFMN oral classification v1.0.2 model predicts pentylene glycol to be a carcinogen with low confidence. The ADI is 0, indicating that the prediction is not reliable (Appendix D).
    - IRFMN inhalation classification v1.0.2 model predicts pentylene glycol to be a **non-carcinogen** with high confidence. The ADI is **0.941**, indicating that the prediction is reliable (Appendix D).
- Toxtree 2018
  - Pentylene glycol does not contain a structural alert for genotoxic or nongenotoxic carcinogenicity (Appendix E).
- DTU 2024
  - Danish (Q)SAR Database for the CAS number 5343-92-0 reports that pentylene glycol is in the domains of six of the seven of the E Ultra FDA RCA cancer databases and is predicted to be negative for carcinogenicity in all six databases (female rat, rat, male mouse, female mouse, mouse, and rodent). Pentylene glycol is in the domain of one of the seven Leadscope FDA RCA cancer databases, and is predicted it to be negative for carcinogenicity in the this database (female rat). Regarding the liver specific cancer in rat or mouse model, pentylene glycol is within the domain of two models (CASE Ultra and SciQSAR) and the overall battery, and is predicted to be negative in all three (Appendix F).
- U.S. EPA 2019, 2021
  - Attempts were made to evaluate the carcinogenic potential of pentylene glycol using the most current version of OncoLogic (v9.0); however, OncoLogic indicated that its chemical

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class is not supported in the current version of software. Since the knowledge base used in this version of the program has not changed from the last version, ToxServices used the previous version (v8.0) to evaluate the carcinogenic potential of pentylene glycol. ToxServices evaluated this chemical as an aliphatic alcohol. Low molecular weight alcohols (C < 6) are of carcinogenic concern because of possible oxidation to reactive aldehydes. In addition, low molecular weight alcohols with (i) a terminal double bond or Cl/Br/I, (ii) α,β-unsaturation, or (iii) monosubstitution with Cl/Br/I at the α-carbon are of concern as potential genotoxic carcinogens. As pentylene glycol does not have any of these features, and was negative for genotoxicity in *in vitro* assays (see genotoxicity section below), it has a low concern for carcinogenicity (Appendix G).

- Based on a weight of evidence, a score of Low was assigned. The surrogate propylene was negative for carcinogenicity in multiple chronic assays in animals. Pentylene glycol does not contain structural alerts for genotoxic or non-genotoxic carcinogenicity according to Toxtree. Two of the six models in VEGA produced a reliable prediction for carcinogenicity for pentylene glycol, and it was predicted to be a non-carcinogen in both models. Danish QSAR modeling database gave consistently negative predictions for carcinogenicity. OncoLogic suggests a low concern for carcinogenicity. The weight of evidence from surrogate experimental data and from rule-based (VEGA, Toxtree, and OncoLogic) and statistical-based (Danish QSAR) modeling programs indicates that pentylene glycol is not likely to be carcinogenic.

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

Pentylene glycol was assigned a score of Low for mutagenicity/genotoxicity based on consistently negative results in *in vitro* genotoxicity studies with pentylene glycol. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data are available for both gene mutations and chromosome aberrations, and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *In vitro:* Pentylene glycol was negative for mutagenicity in a GLP-compliant bacterial reverse mutation assay conducted according to OECD Guideline 471. *Salmonella typhimurium* strains TA1535, TA1537, TA98, and TA100 were exposed to pentylene glycol (99.5% purity) in water at concentrations of 20, 100, 500, 2,500, and 5,000 µg/plate with and without metabolic activation (Aroclor 1254 rat liver S9 mix). Positive controls were 2-aminoanthracene, methyl-N'-nitro-N-nitrosoguanidine, 4-nitro-o-phenylendiamine, and 9-aminoacridine. There was no cytotoxicity reported. There were no increases in the frequency of revertants with treatment. Vehicle, untreated negative, and positive controls were reported to be valid (Klimisch 1, reliable without restriction).
  - *In vitro:* Pentylene glycol was negative for mutagenicity in a bacterial reverse mutation assay conducted according to OECD Guideline 471 (GLP status not specified). *S. typhimurium* strains TA1535, TA1537, TA98, TA100, and TA1538 were exposed to pentylene glycol (purity and vehicle not reported) at concentrations of 0.32-200 µL/plate with and without metabolic activation (S9-homgenate) in experiment 1 and 0.24-150 µL/plate with and without metabolic activation (S9-homogenate) in experiment 2. Cytotoxicity was reported at concentrations of 200 µL/plate. There were no increases in the frequency of revertants with treatment. Vehicle, untreated negative, and positive controls were not specified (Klimisch 2, reliable with restrictions).

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- *In vitro:* Pentylene glycol was negative for mutagenicity in a GLP-compliant mammalian cell gene mutation assay conducted according to OECD Guideline 476. Mouse lymphoma L5178Y cells were exposed to pentylene glycol (purity and vehicle not reported) at concentrations of 65.3, 130.5, 261, 522, and 1,044 µg/mL with and without metabolic activation (mammalian microsomal fraction S9 mix). Positive controls were methylmethanesulfonate and cyclophosphamide. There was no cytotoxicity reported. There were no increases in the frequency of mutants with treatment. Untreated negative and positive controls were reported to be valid (Klimisch 1, reliable without restriction).
- *In vitro:* Pentylene glycol was negative for clastogenicity in a GLP-compliant chromosome aberration assay conducted according to OECD Guideline 473. Mammalian lymphocytes were exposed to pentylene glycol (purity and vehicle not reported) at concentrations of 339.6, 594.3, and 1,040 µg/mL with and without metabolic activation (mammalian microsomal fraction S9 mix). Positive controls were ethylmethanesulphonate and cyclophosphamide. There was no cytotoxicity reported. There were no increases in the frequency of cells with chromosomal aberrations with treatment. Untreated negative and positive controls were reported to be valid (Klimisch 1, reliable without restriction).

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

Pentylene glycol was assigned a score of Low for reproductive toxicity based on the lack of adverse effects on reproduction in an OECD Guideline 422 combined repeated dose toxicity study with reproduction/developmental toxicity screening test in rats with the surrogate 1,2-butanediol, and lack of effect to male sperm parameters in a dermal repeated dose toxicity study in rats with the surrogate 1,2-hexanediol. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is primarily based on a screening study (OECD Guideline 422).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *Oral: Surrogate: 1,2-Butanediol (CAS #584-03-2)*: In a GLP-compliant combined repeated dose toxicity study with reproduction/developmental toxicity screening test conducted according to OECD Guideline 422, male and female Crj: CD(SD) rats (10/sex/dose group) were administered 1,2-butanediol (>99% purity) in water at doses of 0, 40, 200, or 1,000 mg/kg/day via gavage. Male rats were exposed for 42 days. Reproductive phase females were dosed from two weeks prior to mating to day 3 of lactation (total of 37 days). There were no mortalities and no adverse effects on body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals. There was no effect on reproduction/developmental parameters of copulation, implantation, pregnancy, parturition, and lactation. There were no developmental toxicities. The study authors identified a reproductive toxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, based on a lack of effects (Klimisch 2, reliable with restrictions).
  - *Dermal: Surrogate: 1,2-Hexanediol (CAS #6920-22-5):* In a GLP-compliant subchronic dermal toxicity study conducted according to OECD Guideline 411, male and female Sprague-Dawley rats (15/sex/dose) were administered 1,2-hexanediol (purity not reported) in water at doses of 0, 350, 700, and 1,000 mg/kg/day for 90 days. Male animals were evaluated for sperm motility, total sperm count, and sperm morphology. There were no adverse effects on these parameters in treated males (Klimisch 2, reliable with restrictions).

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Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): L
Pentylene glycol was assigned a score of Low for developmental toxicity based on lack of adverse effects in an OECD Guideline 414 prenatal developmental toxicity study in rats with the surrogate 1,2-hexanediol and in an OECD Guideline 422 combined repeated dose toxicity study with reproduction/developmental toxicity screening test in rats with the surrogate 1,2-butanediol. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for strong surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *Oral: Surrogate: 1,2-Hexanediol (CAS #6920-22-5):* In a GLP-compliant prenatal developmental toxicity study conducted according to OECD Guideline 414, pregnant female Crl: CD (SD) IGS BR rats (24/dose) were administered 1,2-hexanediol (purity and vehicle not reported) at doses of 0, 30, 100, and 300 mg/kg/day via gavage on gestation days (GD) 5-19. Animals were sacrificed on GD 20. There were no treatment-related effects on numbers of live litters, implantations, resorptions, live and dead fetuses, sex ratio of the fetuses, average fetus weight, or fetal external examinations. The study authors assigned a maternal and developmental toxicity NOAEL of 300 mg/kg/day, the highest dose tested, based on a lack of effects (Klimisch 2, reliable with restrictions).
  - *Oral: Surrogate: 1,2-Butanediol (CAS #584-03-2)*: In a GLP-compliant combined repeated dose toxicity study with reproduction/developmental toxicity screening test conducted according to OECD Guideline 422, male and female Crj: CD(SD) rats (10/sex/dose group) were administered 1,2-butanediol (>99% purity) in water at doses of 0, 40, 200, or 1,000 mg/kg/day via gavage. Male rats were exposed for 42 days. Reproductive phase females were dosed from two weeks prior to mating to day 3 of lactation (total of 37 days). There were no mortalities and no adverse effects on body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals. There was no effect on reproduction/developmental parameters of copulation, implantation, pregnancy, parturition, and lactation. There were no developmental toxicities. The study authors identified a developmental toxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, based on a lack of effects (Klimisch 2, reliable with restrictions).

Endocrine Activity (E) Score (H, M, or L): DG
Pentylene glycol was assigned a score of Data Gap for endocrine activity based on insufficient data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2024
  - Pentylene glycol was inactive for estrogen receptor agonism, antagonism, and binding using the CERAPP Potency Level (from literature) models in ToxCast (Appendix H).

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Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen® Guidance v1.4, Annex 2 for more details.

Acute Mammalian Toxicity (AT) (Group II) Score (vH, H, M, or L): L

Pentylene glycol was assigned a score of Low for acute toxicity based on oral LD_{50} values > 2,000 mg/kg in rats, mice, rabbits, and guinea pigs, a dermal LD_{50} > 2,000 mg/kg in rats, and a 4-hour aerosol inhalation LC_{50} > 7.015 mg/L in rats. 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 5 mg/L for dusts/mists/fumes (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *Oral:* LD_{50} (male and female Tif:RAIf (SPF) rats) > 5,000 mg/kg (non-GLP, OECD Guideline 401) (Klimisch 2, reliable with restrictions)
  - *Dermal:* LD_{50} (male and female Tif:RAIf (SPF) rats) > 2,000 mg/kg (non-GLP, OECD Guideline 402) (Klimisch 2, reliable with restrictions)
  - *Inhalation:* 4-hour aerosol LC_{50} (male and female Tif:RAIf (SPF) rats) > 7,015 mg/m^3 (7.015 mg/L) (non-GLP, similar to OECD Guideline 403) (Klimisch 2, reliable with restrictions)
- RTECS 2011, CIR 2012, PubChem 2024
  - *Oral:* LD_{50} (rat, sex and strain not specified) = 12,700 mg/kg
  - *Oral:* LD_{50} (mouse, sex and strain not specified) = 7,400 mg/kg
  - *Oral:* LD_{50} (rabbit, sex and strain not specified) = 3,700 mg/kg
  - *Oral:* LD_{50} (guinea pig, sex and strain not specified) = 5,200 mg/kg

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) (Group II) Score (vH, H, M, or L): L

Pentylene glycol was assigned a score of Low for systemic toxicity (single dose) based on a lack of specific target organ toxicity in acute oral, dermal, and inhalation toxicity studies in rats with pentylene glycol. Transient clinical signs of toxicity were evaluated separately under single exposure neurotoxicity. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (single dose) when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* GHS – New Zealand – Aspiration hazard Category 1.
- ECHA, CAS #5343-92-0, 2024
  - *Oral:* In a non-GLP-compliant acute oral toxicity study conducted according to OECD Guideline 401, male and female Tif:RAIf (SPF) rats (5/sex/dose) were administered pentylene glycol (purity not reported) in water at a dose of 5,000 mg/kg via gavage and observed for 14 days. There were no mortalities and no adverse effects on body weights. Clinical signs included sedation (up to 5 hours after administration), dyspnea (up to 12 days after administration), exophthalmos (up to 11 days after administration), ruffled fur (up to 8

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days after administration), and a curved body position (up to 7 days after administration). There were no adverse effects at necropsy (Klimisch 2, reliable with restrictions).
    - *Dermal:* In a non-GLP-compliant acute dermal toxicity study conducted according to OECD Guideline 402, male and female Tif:RAIf (SPF) rats (5/sex/dose) were administered unchanged pentylene glycol (purity not reported) to the skin at a dose of 2,000 mg/kg for 24 hours under occlusive conditions. There were no mortalities and no adverse effects on body weights. Clinical signs included sedation (up to 5 hours after administration), dyspnea (up to 8 days after administration), exophthalmos (up to 7 days after administration), ruffled fur (up to 8 days after administration), and erythema and edema. There were no adverse effects at necropsy (Klimisch 2, reliable with restrictions).
    - *Inhalation:* In a non-GLP-compliant acute inhalation toxicity study conducted similar to OECD Guideline 403, male and female Tif:RAIf (SPF) rats (10/sex/concentration) were exposed nose only to pentylene glycol (purity not reported) aerosol in air at concentrations of 3,380 and 7,015 mg/m^3 for 4 hours. There were no mortalities and no adverse effects on body weight. Clinical signs included dyspnea, ruffled fur, and curved body position up to 1 day after treatment. Mottled or reddish lungs was noted at necropsy in some animals (Klimisch 2, reliable with restrictions).
    - Pentylene glycol has a kinematic viscosity of 24 mm^2/s at 40°C in a GLP-compliant OECD Guideline 114 assay (Klimisch 1, reliable without restriction).
        - *GHS criteria classify chemicals as aspiration hazards Category 1 or 2 when they are hydrocarbons, alcohols or ketones with a kinematic viscosity of ≤ 20.5 or ≤ 14 mm^2/s at 40°C, respectively, along with consideration of surface tension, water solubility, boiling point and volatility (UN 2023). Although pentylene glycol is a diol with 5 carbons, it has a kinematic viscosity of 24 mm^2/s at 40°C. Therefore, a GHS classification for aspiration hazard is not warranted.*
- CCID 2024
    - No rationale for classification to GHS Category 1 for aspiration in New Zealand is provided.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) Score (H, M, or L): L

Pentylene glycol was assigned a score of Low for systemic toxicity (repeated dose) based on an oral NOAEL of 1,000 mg/kg/day in a 90-day study in rats with pentylene glycol and a dermal NOAEL of 1,000 mg/kg/day in a 90-day study in rats with the surrogate 1,2-hexanediol. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when the oral LOAEL is greater than 100 mg/kg/day for 90-day studies and the dermal LOAEL is greater than 200 mg/kg/day for 90-days studies (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance and a strong surrogate.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
    - *Oral:* In a GLP-compliant 90-day repeated dose toxicity study conducted according to OECED Guideline 408, male and female Wistar rats (10/sex/dose) were administered pentylene glycol (99.7% purity) in water at doses of 0, 50, 150, and 1,000 mg/kg/day via gavage for 91 (males) or 92 (females) days. There were no mortalities or clinical signs of toxicity reported, and there were no adverse effects on body weight, food consumption and efficiency, hematology parameters, clinical chemistry parameters, urinalysis, organ weight, or pathological examination between the treated and control animals. The study authors

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identified a systemic toxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, based on a lack of effects (Klimisch 1, reliable without restriction).

- *Oral:* Surrogate: 1,2-Butanediol (CAS #584-03-2): In a GLP-compliant combined repeated dose toxicity study with reproduction/developmental toxicity screening test conducted according to OECD Guideline 422, male and female Crj: CD(SD) rats (10/sex/dose group) were administered 1,2-butanediol (>99% purity) in water at doses of 0, 40, 200, or 1,000 mg/kg/day via gavage. Male rats were exposed for 42 days. Females were dosed from two weeks prior to mating to day 3 of lactation (total of 37 days). There were no mortalities and no adverse effects on body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals. The study authors identified a systemic toxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, based on a lack of effects (Klimisch 1, reliable without restriction).
  - *Based on the 37-day duration of treatment for females in this study, the guidance values were multiplied by 2.4 (i.e., 100 mg/kg/day * 2.4 = 240 mg/kg/day), as 90-days is approximately 2.4 times the duration of 37-days.*
- *Dermal:* Surrogate: 1,2-Hexanediol (CAS #6920-22-5): In a GLP-compliant subchronic dermal toxicity study conducted according to OECD Guideline 411, male and female Sprague-Dawley rats (15/sex/dose) were administered 1,2-hexanediol (purity not reported) in water at doses of 0, 350, 700, and 1,000 mg/kg/day for 90 days. There were no mortalities. Clinical signs included rough coat, fur staining, and slight dermal irritation at 1,000 mg/kg/day. Slight body weight decreases were noted in high dose males; however, they were not considered to be toxicologically relevant. There were no toxicologically relevant effects on hematology parameters or clinical chemistry parameters. Changes in urinalysis parameters were considered to be non-adverse. There were slight changes in heart and kidney weights, however, there were no associated histopathological alternations. The study authors identified a systemic toxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, based on a lack of toxicologically significant adverse effects (Klimisch 2, reliable with restrictions).

- CIR 2012, RTECS 2011
  - *Oral:* A TD_{Lo} of 2,450 mg/kg is reported following intermittent oral administration of pentylene glycol to rats over a 28-week period. No further details were provided.

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): *M*
Pentylene glycol was assigned a score of Moderate for neurotoxicity (single dose) based on the reversible behavioral/neurological clinical signs of toxicity detected following single oral, dermal, and inhalation doses of pentylene glycol, in combination with the acute solvent syndrome information, leading to ToxServices conservatively classifying pentylene glycol as a GHS Category 3 specific target organ toxicant following single exposures for narcotic effects. GreenScreen® criteria classify chemicals as a Moderate hazard for neurotoxicity (single dose) when a GHS Category 3 classification for transient narcotic effects is warranted (CPA 2018b). The confidence in the score is low as it is unclear if these effects have a neurological etiology or are merely reflective of general signs of discomfort.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *Oral:* In a non-GLP-compliant acute oral toxicity study conducted according to OECD Guideline 401, male and female Tif:RAIf (SPF) rats (5/sex/dose) were administered

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pentylene glycol (purity not reported) in water at a dose of 5,000 mg/kg via gavage and observed for 14 days. There were no mortalities. Clinical signs included sedation (up to 5 hours after administration), dyspnea (up to 12 days after administration), exophthalmos (up to 11 days after administration), ruffled fur (up to 8 days after administration), and a curved body position (up to 7 days after administration). There were no adverse effects at necropsy (Klimisch 2, reliable with restrictions).

- *Dermal:* In a non-GLP-compliant acute dermal toxicity study conducted according to OECD Guideline 402, male and female Tif:RAIf (SPF) rats (5/sex/dose) were administered unchanged pentylene glycol (purity not reported) to the skin at a dose of 2,000 mg/kg for 24 hours under occlusive conditions. There were no mortalities. Clinical signs included sedation (up to 5 hours after administration), dyspnea (up to 8 days after administration), exophthalmos (up to 7 days after administration), and ruffled fur (up to 8 days after administration). There were no adverse effects at necropsy (Klimisch 2, reliable with restrictions).
- *Inhalation:* In a non-GLP-compliant acute inhalation toxicity study conducted similar to OECD Guideline 403, male and female Tif:RAIf (SPF) rats (10/sex/concentration) were exposed nose only to pentylene glycol (purity not reported) aerosol in air at concentrations of 3,380 and 7,015 mg/m^3 for 4 hours. There were no mortalities. Clinical signs included dyspnea, ruffled fur, and curved body position up to 1 day after treatment. Mottled or reddish lungs was noted at necropsy in some animals (Klimisch 2, reliable with restrictions).

- PubChem 2024
  - Pentylene glycol is associated with acute solvent syndrome.

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

Pentylene glycol was assigned a score of Low for neurotoxicity (repeated dose) based on lack of effects in a functional observational battery (FOB) at oral doses up to 1,000 mg/kg/day in an 90-day study in rats with pentylene glycol and lack of effects in behavioral examinations at dermal doses up to 1,000 mg/kg/day in a 90-day study in rats with the surrogate 1,2-hexandiol. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when the oral neurotoxicity LOAEL is greater than 100 mg/kg/day for 90-day studies and the dermal neurotoxicity LOAEL is greater than 200 mg/kg/day for 90-days studies (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance and a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - *Oral:* In the previously described GLP-compliant 90-day repeated dose toxicity study conducted according to OECED Guideline 408, male and female Wistar rats (10/sex/dose) were administered pentylene glycol (99.7% purity) in water at doses of 0, 50, 150, and 1,000 mg/kg/day via gavage for 91 (males) or 92 (females) days. An FOB as well as measurement of motor activity (MA) were carried out at the end of the administration period. There were no adverse effects reported. Thus a neurotoxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, can be established for this study based on a lack of effects (Klimisch 1, reliable without restriction).
  - *Dermal: Surrogate: 1,2-Hexanediol (CAS #6920-22-5):* In a GLP-compliant subchronic dermal toxicity study conducted according to OECD Guideline 411, male and female Sprague-Dawley rats (15/sex/dose) were administered 1,2-hexanediol (purity not reported) in water at doses of 0, 350, 700, and 1,000 mg/kg/day for 90 days. Hand-held and open-field

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observations were performed weekly and animals were evaluated for elicited behaviors (forelimb and hindlimb grip strength and tail flick) during the last week of the study. Ther were no adverse effects on these parameters. A neurotoxicity NOAEL of 1,000 mg/kg/day, the highest dose tested, can be established based on a lack of adverse effects (Klimisch 2, reliable with restrictions).

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

Pentylene glycol was assigned a score of Low for skin sensitization based on negative results for skin sensitization in an OECD Guideline 406 Maurer optimization test in guinea pigs with pentylene glycol. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol was not sensitizing to the skin in a non-GLP-compliant Maurer optimization test conducted according to OECD Guideline 406. Male and female Pirbright white guinea pigs (10/sex) received intradermal induction with 0.1 mL of a 0.1% solution of pentylene glycol (purity not reported) in physiological saline; during the second and third week of the induction the test material was incorporated in a mixture of the normal vehicle with Bacto adjuvant (1:1). Animals received an intradermal challenge of 0.1 mL of a 0.1% solution in saline or epicutaneous challenge of 10% in Vaseline for 24 hours under occlusive conditions. There were no positive responses in treated animals at 24 hours after challenge (Klimisch 2, reliable with restrictions).
  - A 50% aqueous solution of a commercially-available pentylene glycol product (containing an unknown percentage of active ingredient) was not irritating or sensitizing to the skin of 53 human volunteers in a human repeat insult patch test (HRIPT) (Klimisch 2, reliable with restrictions).

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): *L*

Pentylene glycol was assigned a score of Low for respiratory sensitization based on a lack of skin sensitization potential according to ECHA (2017)'s guidance on respiratory sensitization. GreenScreen® criteria classify chemicals as a Low hazard for respiratory sensitization when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is low as this evaluation does not include non-immunologic mechanisms of respiratory sensitization, and no specific data are available for respiratory sensitization.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2023
  - Pentylene glycol does not contain any structural alerts for respiratory sensitization (Appendix I)
- Based on the weight of evidence and guidance from ECHA regarding assessment of respiratory sensitization potential, a score of Low was assigned. The guidance from ECHA states that the mechanisms leading to respiratory sensitization are essentially similar to those leading to skin sensitization (ECHA 2017). ECHA recommended that if a chemical is not a dermal sensitizer based on high quality data, it is unlikely to be a respiratory sensitizer. ECHA also noted that this rationale

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does not cover respiratory hypersensitivity caused by non-immunological mechanisms, for which human experience is the main evidence of activity (ECHA 2017). As pentylene glycol was not sensitizing to the skin (see skin sensitization section above), and a literature search did not find any human evidence of respiratory sensitization by pentylene glycol, and as pentylene glycol does not contain any structural alerts for respiratory sensitization (OECD 2023), pentylene glycol is not expected to be a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): L

Pentylene glycol was assigned a score of Low for skin irritation/corrosivity based on negative results for skin irritation in two acute dermal irritation assays in rabbits with pentylene glycol. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol was not irritating to the skin in a GLP-compliant acute dermal irritation assay conducted according to OECD Guideline 404. In this assay, 0.5 mL unchanged pentylene glycol (>99% purity) was applied to clipped skin of Vienna white rabbits (n=3) for 4 hours under semi-occlusive conditions. The mean 24, 48, and 72 hours erythema and edema scores were both 0/4 (Klimisch 1, reliable without restriction).
  - Pentylene glycol was not irritating to the skin in an acute dermal irritation assay conducted according to EPA OPP 81-5 (GLP status not specified). In this assay, 0.5 mL pentylene glycol (purity and vehicle not specified) was applied to intact and abraded skin of New Zealand white rabbits (3/sex) for 24 hours under occlusive conditions. The mean 24 and 72 hours erythema and edema scores were 1.1/ and 0.75/4, respectively, for intact skin and 1.1/4 and 0.75/4, respectively, for abraded skin. The primary dermal irritation index was 1.85 (Klimisch 2, reliable with restrictions).

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

Pentylene glycol was assigned a score of Very High for eye irritation/corrosivity based on irreversible effects to the eye after 20 days in an OECD Guideline 404 acute dermal irritation assay in rabbits with pentylene glycol, classifying it to GHS Category 1. GreenScreen® criteria classify chemicals as a Very High hazard for eye irritation/corrosivity when they cause irreversible effects to the eyes and a GHS Category 1 classification is warranted (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol was irritating to the eye in a GLP-compliant acute ocular irritation assay conducted according to OECD Guideline 405. One eye of Vienna white rabbits (n=3) was instilled with 0.1 mL unchanged pentylene glycol (>99% purity) and observed for 21 days. The mean 24, 48 and 72 hours corneal opacity, iris, conjunctivae, and chemosis scores were 1, 0.7, 2.3, and 1.3, respectively in animal 1; 1, 1, 2.1, and 2.0, respectively in animal 2; and 1, 0.8, 2.6, and 1.8, respectively, in animal 3. Effects were not fully reversible in 21 days (Klimisch 1, reliable without restriction).

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        - *Based on GHS guidance (UN 2023), a GHS Category 1 classification is warranted when, in at least one animal, effects on the cornea, iris, or conjunctivae have not fully reversed within an observation period of 21 days.*
    - Pentylene glycol was irritating to the eye in an acute ocular irritation assay conducted according to EPA OPP 81-4 (GLP status not specified). One eye of New Zealand white rabbits (n=9) was instilled with 0.1 mL unchanged pentylene glycol (purity not reported) and observed for 7 days. Eyes were washed 30 seconds after exposure in 3 animals; the eyes of the 6 remaining animals were left unwashed. The primary irritation index was 31.7 for unrinsed eyes and 25.5 for rinsed eyes. Reversibility of effects was not specified (Klimisch 2, reliable with restrictions).

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): L
Pentylene glycol was assigned a score of Low for acute aquatic toxicity based on L/EC_{50} values > 100 mg/L in all three trophic levels. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute aquatic toxicity values are greater than 100 mg/L in all three trophic levels (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for the target substance.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
    - 96-hour LC_{50} (*Danio rerio*, zebrafish) > 1,096 mg/L (measured) (GLP, OECD Guideline 203) (Klimisch 1, reliable without restriction).
    - 48-hour mobility EC_{50} (*Daphnia magna*, daphnia) > 500 mg/L (nominal) (non-GLP, EU Directive 79/831/EWG Appendix V, part C) (Klimisch 2, reliable with restrictions).
    - 72-hour growth rate EC_{50} (*Desmodesmus subspicatus*, green algae) = 9,334.69 mg/L (nominal) (non-GLP, DIN 38412 part 9) (Klimisch 2, reliable with restrictions).

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *L*
Pentylene glycol was assigned a score of Low for chronic aquatic toxicity based on chronic aquatic toxicity values (experimental and modeled) > 10 mg/L in all three trophic levels. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when chronic aquatic toxicity values are greater than 10 mg/L (CPA 2018b). The confidence in the score is low as it is partially based on modeling and experimental data were not available for all three trophic levels.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
    - 72-hour growth rate EC_{10} (*D. subspicatus*, green algae) = 5,477.33 (nominal) (non-GLP, DIN 38412 part 9) (Klimisch 2, reliable with restrictions).
- U.S. EPA 2022
    - Pentylene glycol belongs to the neutral organics ECOSAR chemical class. The most conservative predicted chronic values (ChVs) are 284 mg/L in fish, 104 mg/L in daphnia, and 115 mg/L in green algae (Appendix J).

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Environmental Fate (Fate)

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

Pentylene glycol was assigned a score of Low for persistence based on the results of an OECD Guideline 301 E assay indicating it meets the pass level, but not the 10-day window. Therefore, it does not meet the current GHS rapid degradability criteria (UN 2023). Therefore, ToxServices relied on the modeled half-life of 17.3 days in its major compartment, soil, to score this endpoint. GreenScreen® criteria classify chemicals as a Moderate hazard for persistence when the half-life is between 16 and 60 days in soil or sediment (CPA 2018b). The confidence in the score is low as it is based on modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol was readily biodegradable but failed the 10-day window in a non-GLP-compliant OECD Guideline 301 E ready biodegradability (modified OECD screening test) assay. In this assay, 20 mg/L pentylene glycol (purity not reported) was exposed to a mixture of secondary effluent from a sewage treatment plant, the river Rhine and suspension of garden soil for 28 days. The test substance degraded 42% in 7 days, 64% in 14 days, 66% in 21 days, 71% in 27 days, and 73% in 28 days. The 10-day window was therefore not met (Klimisch 2, reliable with restrictions).
  - Pentylene glycol was inherently biodegradable in a non-GLP-compliant inherent biodegradability (Zahn-Wellens/EMPA test) assay conducted in a manner similar to OECD Guideline 302 B. In this assay, 400 mg/L pentylene glycol (purity not reported) was exposed to aerobic, industrial, activated sludge (Adaption not specified) for 28 days. The test substance degraded 11% in 3 hours, 23% in 1 day, 82% in 3 days, and 95% in 8 days (Klimisch 2, reliable with restrictions).
- U.S. EPA 2017
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that pentylene glycol is expected to be readily biodegradable. Fugacity modeling (MCI method) predicts 57% will partition to soil with a half-life of 17.3 days, 40.8% will partition to water with a half-life of 8.7 days, and 2.1% will partition to air with a half-life of 14.8 hours, and 0.0722% will partition to sediment with a half-life of 77.9 days (Appendix K).
- Based on the weight of evidence, a low confidence score of Moderate was assigned. A reliable, OECD Guideline 301E study with the target compound indicates pentylene glycol is readily biodegradable, but it did not meet the 10-day window in this study. An inherent biodegradability test (the Zahn-Wellens/EMPA test) indicates pentylene glycol has potential for ultimate biodegradation as it degraded more than 70% in 7 days; however, the optimum conditions in inherent biodegradability tests increase biodegradation potential and positive results should not be interpreted as evidence of GHS rapid degradation in the environment (UN 2023). Thus, the experimental biodegradation results for the target substance do not support a score of Very Low (i.e., meeting the 10-day window) or Low (GHS rapidly degradable) for this endpoint. Fugacity modeling using EPI Suite™ was included in order to identify the dominant environmental compartment(s) the chemical will partition to, as no experimental partitioning data were available. Fugacity modeling predicts the dominant compartment is soil and the half-life in this compartment was predicted to be between 16 and 60 days, which corresponds to a score of Moderate. Although the half-life is < 14 days in the OECD Guideline 301E study, this study performed in water, and no biodegradation data in soil (the dominant compartment) were identified. Taken all together, a low

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confidence score of Moderate was assigned based on the modeled half-life of 17.3 days in its major compartment, soil, as additional data may indicate a lower score is warranted.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
Pentylene glycol was assigned a score of Very Low for bioaccumulation based on a measured log K_{ow} of 0.06 and an estimated BCF of 0.9145. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when they log K_{ow} is less than 4 and the BCF is less than 100 (CPA 2018b). The confidence in the score is high as it is based on a measured log K_{ow} with support from modeling.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol has a measured log K_{ow} of 0.06 in a non-GLP-compliant shake-flask method test (Klimisch 2, reliable with restrictions).
- U.S. EPA 2017
  - BCFBAF predicts a BCF of 3.162 L/kg wet-wt using the regression based model based on a measured log K_{ow} of 0.06, and a BCF of 0.9415 using the Arnot-Gobas model for the upper trophic level, taking metabolism into consideration (Appendix K).

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Pentylene glycol was assigned a score of Low for reactivity based on it not being explosive or oxidizing and its stability/physical hazard ratings of 0 from NFPA and HMIS. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is low due to the lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #5343-92-0, 2024
  - Pentylene glycol does not contain chemical groups associated with explosive properties.
  - Pentylene glycol is incapable of reacting exothermically with combustible materials on the basis of chemical structure.
- Santa Cruz Biotechnology 2022
  - An SDS for pentylene glycol (>98% purity) has a stability rating of 0 from the NFPA ("Normally stable, even under fire exposure conditions, and is not reactive with water") and physical hazard rating of 0 from HMIS ("Materials that are normally stable, even under fire conditions, and will not react with water, polymerize, decompose, condense, or self-react. Non-explosives").

Flammability (F) Score (vH, H, M, or L): L
Pentylene glycol was assigned a score of Low for flammability based on its flash point of 100°C and it not being classified as a flammable liquid under GHS. GreenScreen® criteria classify chemicals as a Low hazard for flammability when adequate data are available and negative and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable measured data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

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- ECHA, CAS #5343-92-0, 2024
    - Pentylene glycol has a flash point of 110°C measured according to DIN 51785 in a closed cup assay (Klimisch 2, reliable with restrictions).
        - *As pentylene glycol has a flash point >93°C, a flammable liquid classification under GHS is not warranted (UN 2023).*

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Use of New Approach Methodologies (NAMs)[9] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in silico* modeling for carcinogenicity, endocrine activity, respiratory sensitization, aquatic toxicity, persistence, and bioaccumulation, and *in vitro* testing for mutagenicity. NAMs are non-animal alternatives that can be used alone or in combination to provide information for safety assessment (Madden et al. 2020). At present, there is not a uniformly accepted framework on how to report and apply individual NAMs (U.S. EPA 2020, OECD 2020). The expanded application of NAMs greatly amplifies the need to communicate uncertainties associated with their use. As defined by EFSA (2018), uncertainty is "a general term referring to all types of limitations in available knowledge that affect the range and probability of possible answers to an assessment question." The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties (OECD 2020):

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

As shown in Table 4, Type I (input data) uncertainties in pentylene glycol's NAMs dataset include lack of/insufficient experimental data for carcinogenicity, endocrine activity, respiratory sensitization, and chronic aquatic toxicity, and lack of validated test methods for respiratory sensitization. Pentylene glycol's Type II (extrapolation output) uncertainties include the lack of defined applicability domains in some modeling programs, limitation of *in vitro* genotoxicity assays in mimicking *in vivo* metabolism, their focusing on one or only a few types of genotoxicity events, the uncertain *in vivo* relevance of *in silico* modeling of receptor reactivity due to lack of consideration of toxicokinetics, and the limitation of OECD Toolbox in identifying structural alerts for respiratory sensitization without accounting for non-immunologic mechanisms of respiratory sensitization.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses

Uncertainty Analyses (OECD 2020)	
Type I Uncertainty: Data/Model Input	**Carcinogenicity**: No experimental data are available on the target chemical. **Endocrine activity**: No experimental data are available. **Respiratory sensitization**: No experimental data are available and there are no validated test methods. **Chronic aquatic toxicity:** No experimental data are available for two trophic levels.
Type II Uncertainty: Extrapolation Output	**Carcinogenicity**: Toxtree only identifies structural alerts (SAs), and no applicability domain can be defined (Toxtree 2018). Only two of the six VEGA models produced reliable (i.e., Global AD index > 0.7) predictions. **Genotoxicity:** The bacterial reverse mutation assay (as defined in OECD Guideline 471) only tests point-mutation inducing activity in non-mammalian cells, and the exogenous metabolic activation

[9] NAMs refers to any non-animal technology, methodology, approach, or combination thereof that inform chemical hazard and risk assessments. NAMs include *in silico*/computational tools, *in vitro* biological profiling (e.g., cell cultures, 2,3-D organotypic culture systems, genomics/transcriptomics, organs on a chip), and frameworks (i.e., adverse outcome pathways (AOPs), defined approaches (DA), integrated approaches to testing and assessment (IATA).

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	system does not entirely mimic *in vivo* conditions[10]. The mammalian cell gene mutation assay (as defined in OECD Guideline 476) only detects gene mutations, and the exogenous metabolic activation system does not entirely mirror *in vivo* metabolism (i.e., the liver S9 mix contains enzymes present in the endoplasmic reticulum but not the cytosol of liver cells).[11] The *in vitro* chromosome aberration assay (OECD Guideline 473) does not measure aneuploidy and it only measures structural chromosomal aberrations. The exogenous metabolic activation system does not entirely mirror *in vivo* metabolism[12]. **Endocrine activity:** ToxCast models don't define applicability domain. The *in vivo* relevance of *in silico* modeling of receptor activities is uncertain due to lack of consideration of toxicokinetics. **Respiratory sensitization**: The OECD Toolbox only identifies structural alerts, and does not define applicability domains. Additionally, the ECHA guidance (2017), on which the use of OECD Toolbox structural alerts is based, does not evaluate non-immunologic mechanisms for respiratory sensitization.	
Endpoint	**NAMs Data Available and Evaluated? (Y/N)**	**Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)**
Carcinogenicity	Y	*In silico* modeling: VEGA/Toxtree/OncoLogic™/Danish QSAR
Mutagenicity	Y	*In vitro* data: Bacterial reverse mutation assay/*in vitro* gene mutation assay/*in vitro* chromosome aberration assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	Y	*In silico* modeling: ToxCast
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	N	

[10] https://www.oecd-ilibrary.org/docserver/9789264071247-en.pdf?expires=1614097593&id=id&accname=guest&checksum=89925F80B9F4BD2FFC6E90F94A0EE427
[11] https://www.oecd-ilibrary.org/docserver/9789264264809-en.pdf?expires=1614097800&id=id&accname=guest&checksum=C0DE371FB9C5A878E66C9AB7F84E6BBE
[12] https://www.oecd-ilibrary.org/docserver/9789264264649-en.pdf?expires=1614098015&id=id&accname=guest&checksum=6A4F9CE52EA974F5A74793DD54D54352

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Respiratory sensitization	Y	*In silico* modeling: OECD Toolbox structural alerts
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	Y	*In silico* modeling: ECOSAR
Persistence	Y	*In silico* modeling: EPI Suite™ Non-animal testing: OECD Guideline 301 and 302 Biodegradation tests
Bioaccumulation	Y	*In silico* modeling: EPI Suite™

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References

Chemical Classification and Information Database (CCID). 2024. 1,2-Pentanediol (CAS #5343-92-2). New Zealand Environmental Protection Authority. Available: https://www.epa.govt.nz/database-search/chemical-classification-and-information-database-ccid/view/A57632DB-8873-4A96-A68A-75B4B7EB66B6

Clean Production Action (CPA). 2018a. GreenScreen® Assessment Expiration Policy. October 2, 2018.

Clean Production Action (CPA). 2018b. The GreenScreen® for Safer Chemicals Guidance. Version 1.4 Guidance. Dated January, 2018. Available: https://www.greenscreenchemicals.org/static/ee_images/uploads/resources/GreenScreen_Guidance_v1_4_2018_01_Final.pdf

Cosmetic Ingredient Review (CIR). 2012. Safety assessment of 1,2-glycols as used in cosmetics. *Int. J. Toxicol.* 31(Suppl. 2): 147S-168S.

Danish Technical University (DTU). 2024. National Food Institute. Danish QSAR Database. Available: http://qsar.food.dtu.dk/.

European Chemicals Agency (ECHA). 2017. Guidance on information requirements and Chemical Safety Assessment. Chapter R.7a: Endpoint specific guidance. Version 6.0. Dated: July 2017. Available: https://echa.europa.eu/documents/10162/17224/information_requirements_r7a_en.pdf/e4a2a18f-a2bd-4a04-ac6d-0ea425b2567f?t=1500286622893

European Chemicals Agency (ECHA). 2024. REACH dossier for Pentane-1,2-diol (CAS #5343-92-0). Available : https://echa.europa.eu/registration-dossier/-/registered-dossier/2101/4/23

European Commission (EC). 2024. CosIng database entry for Pentylene Glycol (CAS #5343-92-0). Available: https://ec.europa.eu/growth/tools-databases/cosing/details/58983

European Food Safety Authority (EFSA). 2018. Guidance on uncertainty analysis in scientific assessments. *EFSA J.* 16(1): e05123. Available: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7009727/

Gad, S. 2016. QSAR Tools for Drug Safety. Chapter 10. In, Drug Safety Evaluation. Third Edition. New York: Wiley. 209-224.

Madden, J.C., S.J. Enoch, A. Paini, and M.T.D. Cronin. 2020. A review of *in silico* tools as alternatives to animal testing: principles, resources, and applications. *Alt. Lab. Animals.* 1-27. Available: https://journals.sagepub.com/doi/pdf/10.1177/0261192920965977

Organisation for Economic Co-operation and Development (OECD). 2020. Overview of Concepts and Available Guidance related to Integrated Approaches to Testing and Assessment (IATA), Series on Testing and Assessment, No. 329, Environment, Health and Safety, Environment Directorate.

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Available: https://www.oecd.org/chemicalsafety/risk-assessment/concepts-and-available-guidance-related-to-integrated-approaches-to-testing-and-assessment.pdf

Organisation for Economic Co-operation and Development (OECD). 2023. OECD QSAR Toolbox for Grouping Chemicals into Categories Version 4.6. Available: https://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm#Download_qsar_application_toolbox

Pharos. 2024. Pharos chemical and material library entry for Pentylene glycol (CAS #5343-92-0). Available: http://www.pharosproject.net/material/.

PubChem. 2024. 1,2-Pentanediol (CAS #5343-92-0). United States National Library of Medicine. Available: https://pubchem.ncbi.nlm.nih.gov/

Registry of Toxic Effects of Chemical Substances (RTECS). 2011. 1,2-Pentanediol (CAS #5343-92-0). Available: https://chemical-search.toxplanet.com/

Sahigara, F. 2007. Defining the Applicability Domain of QSAR models: An overview. Available: http://www.moleculardescriptors.eu/tutorials/T7_moleculardescriptors_ad.pdf

Santa Cruz Biotechnology. 2022. Safety data sheet for 1,2-Pentanediol. Version 1. Dated December 15, 2022. Available: https://www.scbt.com/p/1-2-pentanediol-5343-92-0

ToxServices. 2021. SOP 1.37: GreenScreen® Hazard Assessments. Dated: May 24, 2021.

Toxtree. 2018. Estimation of Toxic Hazard- A Decision Tree Approach v3.1.0. Available: http://toxtree.sourceforge.net.

United Nations (UN). 2023. Globally Harmonized System of Classification and Labelling of Chemicals (GHS). Tenth revised edition.

United Nations Environment Programme (UNEP). 2001. Screening Information Dataset (SIDS) for propylene glycol (CAS #57-55-6). Organisation for Economic Co-operation and Development (OECD). Available at: http://www.inchem.org/documents/sids/sids/57-55-6.pdf

United States Department of Transportation (U.S. DOT). 2008a. Chemicals Listed with Classification. 49 CFR § 172.101. Available: http://www.gpo.gov/fdsys/pkg/CFR-2008-title49-vol2/pdf/CFR-2008-title49-vol2-sec172-101.pdf.

United States Department of Transportation (U.S. DOT). 2008b. Classification Criteria. 49 CFR § 173. Available: http://www.ecfr.gov/cgi-bin/text-idx?c=ecfr&tpl=/ecfrbrowse/Title49/49cfr173_main_02.tpl

United States Environmental Protection Agency (U.S. EPA). 2015. Safer Choice Standard. Available: https://www.epa.gov/saferchoice/standard

United States Environmental Protection Agency (U.S. EPA). 2017. Estimation Programs Interface (EPI) Suite™ Web, v4.11, Washington, DC, USA. Available: http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm.

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United States Environmental Protection Agency (U.S. EPA). 2019. OncoLogic™. Version 8.0.16 Washington, DC, USA.

United States Environmental Protection Agency (U.S. EPA). 2020. New Approach Methods Workplan. Office of Research and Development. Office of Chemical Safety and Pollution Prevention. EPA 615B20001. June 2020. Available: https://www.epa.gov/sites/default/files/2020-06/documents/epa_nam_work_plan.pdf

United States Environmental Protection Agency (U.S. EPA). 2021. OncoLogic™. Version 9.0 Washington, DC, USA.

United States Environmental Protection Agency (U.S. EPA). 2022. ECOSAR 2.2. Washington, DC, USA. Available: http://www.epa.gov/oppt/newchems/tools/21ecosar.htm/.

United States Environmental Protection Agency (U.S. EPA). 2023. Safer Chemical Ingredients List (SCIL). Available: https://www.epa.gov/saferchoice/safer-ingredients

United States Environmental Protection Agency (U.S. EPA). 2024. CompTox Dashboard. Available: https://comptox.epa.gov/dashboard

Virtual Models for Evaluating the Properties of Chemicals within a Global Architecture (VEGA). 2023. Predictive Model Platform version 1.2.3. Available: https://www.vegahub.eu/download/vega-qsar-download/

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APPENDIX A: Hazard Classification 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

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APPENDIX B: Results of Automated GreenScreen® Score Calculation for Pentylene Glycol (CAS #5343-92-0)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

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	Pentylene Glycol	5343-92-0	L	L	*L*	L	DG	L	L	L	*M*	L	L	*L*	L	vH	L	*L*	*M*	vL	*L*	L

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Pentylene Glycol	2

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

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
Pentylene Glycol	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

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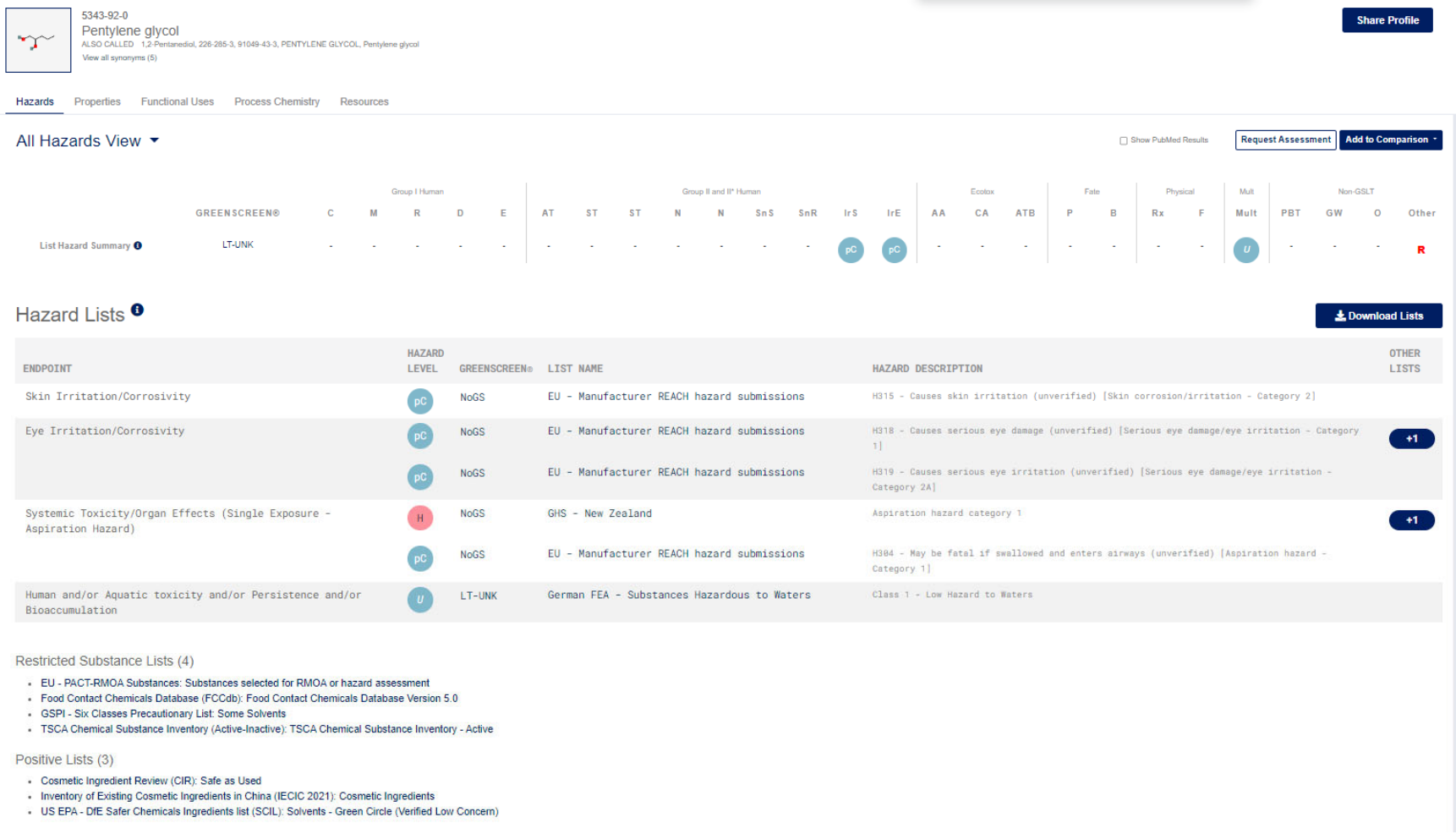
APPENDIX C: Pharos Output for Pentylene Glycol (CAS #5343-92-0)



5343-92-0
Pentylene glycol
ALSO CALLED 1,2-Pentanediol, 226-285-3, 91049-43-3, PENTYLENE GLYCOL, Pentylene glycol
View all synonyms (5)

Share Profile

Hazards | Properties | Functional Uses | Process Chemistry | Resources

All Hazards View

Show PubMed Results | Request Assessment | Add to Comparison

		Group I Human					Group II and II* Human								Ecotox			Fate		Physical		Mult	Non-GSLT			
	GREENSCREEN®	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
List Hazard Summary	LT-UNK	-	-	-	-	-	-	-	-	-	-	-	-	pC	pC	-	-	-	-	-	-	-	U	-	-	-	R

Hazard Lists

Download Lists

ENDPOINT	HAZARD LEVEL	GREENSCREEN®	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Skin Irritation/Corrosivity	pC	NoGS	EU - Manufacturer REACH hazard submissions	H315 - Causes skin irritation (unverified) [Skin corrosion/irritation - Category 2]	
Eye Irritation/Corrosivity	pC	NoGS	EU - Manufacturer REACH hazard submissions	H318 - Causes serious eye damage (unverified) [Serious eye damage/eye irritation - Category 1]	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H319 - Causes serious eye irritation (unverified) [Serious eye damage/eye irritation - Category 2A]	
Systemic Toxicity/Organ Effects (Single Exposure - Aspiration Hazard)	H	NoGS	GHS - New Zealand	Aspiration hazard category 1	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H304 - May be fatal if swallowed and enters airways (unverified) [Aspiration hazard - Category 1]	
Human and/or Aquatic toxicity and/or Persistence and/or Bioaccumulation	U	LT-UNK	German FEA - Substances Hazardous to Waters	Class 1 - Low Hazard to Waters	

Restricted Substance Lists (4)

- EU - PACT-RMOA Substances: Substances selected for RMOA or hazard assessment
- Food Contact Chemicals Database (FCCdb): Food Contact Chemicals Database Version 5.0
- GSPI - Six Classes Precautionary List: Some Solvents
- TSCA Chemical Substance Inventory (Active-Inactive): TSCA Chemical Substance Inventory - Active

Positive Lists (3)

- Cosmetic Ingredient Review (CIR): Safe as Used
- Inventory of Existing Cosmetic Ingredients in China (IECIC 2021): Cosmetic Ingredients
- US EPA - DfE Safer Chemicals Ingredients list (SCIL): Solvents - Green Circle (Verified Low Concern)

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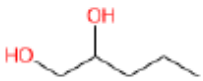
APPENDIX D: VEGA Carcinogenicity Results for Pentylene Glycol (CAS #5343-92-0)

1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value
- predicted substance falls into a neuron that is populated by no compounds of the training set

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Carcinogen activity: Carcinogen
P(Carcinogen): 0.608
P(NON-Carcinogen): 0.392
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

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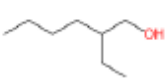
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

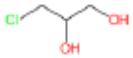
Compound #1

CAS: 57-55-6
Dataset id:677 (Training Set)
SMILES: OCC(O)C
Similarity: 0.905
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



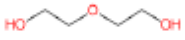
Compound #2

CAS: 104-76-7
Dataset id:314 (Training Set)
SMILES: OCC(CC)CCCC
Similarity: 0.842
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



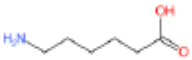
Compound #3

CAS: 96-24-2
Dataset id:349 (Test Set)
SMILES: OCC(O)CCl
Similarity: 0.824
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



Compound #4

CAS: 111-46-6
Dataset id:240 (Training Set)
SMILES: OCCOCCO
Similarity: 0.81
Experimental value : Carcinogen
Predicted value : Carcinogen



Compound #5

CAS: 60-32-2
Dataset id:47 (Training Set)
SMILES: O=C(O)CCCCCN
Similarity: 0.805
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 556-52-5
Dataset id:351 (Training Set)
SMILES: OCC1OC1
Similarity: 0.803
Experimental value : Carcinogen
Predicted value : Carcinogen

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3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
✔	Similar molecules with known experimental value Similarity index = 0.87 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.521 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..
✔	Model class assignment reliability Pos/Non-Pos difference = 0.217 Explanation: model class assignment is well defined..
✖	Neural map neurons concordance Neurons concordance = 0.5 Explanation: predicted substance falls into a neuron that is populated by no compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

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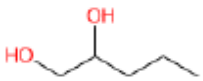
1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

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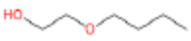
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

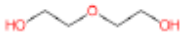


Compound #1

CAS: 111-76-2
Dataset id:596 (Training Set)
SMILES: OCCOCCCC
Similarity: 0.867
Experimental value : Carcinogen
Predicted value : NON-Carcinogen

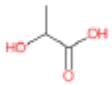
Compound #2

CAS: 107-21-1
Dataset id:306 (Training Set)
SMILES: OCCO
Similarity: 0.83
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #3

CAS: 111-46-6
Dataset id:860 (Training Set)
SMILES: OCCOCCO
Similarity: 0.81
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



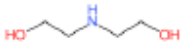
Compound #4

CAS: 814-80-2
Dataset id:815 (Training Set)
SMILES: O=C(O)C(O)C
Similarity: 0.809
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 556-52-5
Dataset id:655 (Training Set)
SMILES: OCC1OC1
Similarity: 0.803
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA7 Epoxides and aziridines



Compound #6

CAS: 111-42-2
Dataset id:600 (Training Set)
SMILES: OCCNCCO
Similarity: 0.78
Experimental value : Carcinogen
Predicted value : NON-Carcinogen

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3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.642 Explanation: The predicted compound is outside the Applicability Domain of the model.
✔	Similar molecules with known experimental value Similarity index = 0.847 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✖	Accuracy of prediction for similar molecules Accuracy index = 0.487 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✖	Concordance for similar molecules Concordance index = 0.487 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

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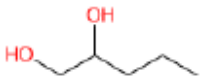
1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is Possible NON-Carcinogen, but the result shows some critical aspects, which require to be checked:
- Accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound could be out of the Applicability Domain of the model
Remarks:
none

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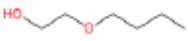
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 111-76-2
Dataset id:498 (Training Set)
SMILES: OCCOCCCC
Similarity: 0.867
Experimental value : Carcinogen
Predicted value : Possible NON-Carcinogen

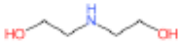
Compound #2

CAS: 107-21-1
Dataset id:667 (Training Set)
SMILES: OCCO
Similarity: 0.83
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #3

CAS: 556-52-5
Dataset id:536 (Training Set)
SMILES: OCC1OC1
Similarity: 0.803
Experimental value : Carcinogen
Predicted value : Carcinogen

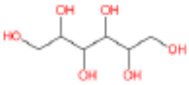
Alerts (not found also in the target): Carcinogenity alert no. 23



Compound #4

CAS: 111-42-2
Dataset id:500 (Training Set)
SMILES: OCCNCCO
Similarity: 0.78
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 34



Compound #5

CAS: 69-65-8
Dataset id:69 (Training Set)
SMILES: OCC(O)C(O)C(O)C(O)CO
Similarity: 0.777
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #6

CAS: 75-65-0
Dataset id:246 (Training Set)
SMILES: OC(C)(C)C
Similarity: 0.772
Experimental value : Carcinogen
Predicted value : Possible NON-Carcinogen

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3.2 Applicability Domain:
Measured Applicability Domain Scores

⚠	Global AD Index AD index = 0.621 Explanation: The predicted compound could be out of the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.83 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.65 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✗	Concordance for similar molecules Concordance index = 0.332 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

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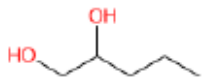
1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is Possible NON-Carcinogen, the result appears reliable.
Anyhow, you should check it through the evaluation of the information given in the following sections.Anyway some issues could be not optimal:
- Accuracy of prediction for similar molecules found in the training set is not optimal

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

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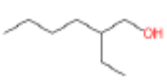
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

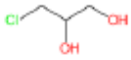
Compound #1

CAS: 57-55-6
Dataset id:677 (Training Set)
SMILES: OCC(O)C
Similarity: 0.905
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #2

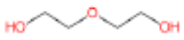
CAS: 104-76-7
Dataset id:314 (Training Set)
SMILES: OCC(CC)CCCC
Similarity: 0.842
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #3

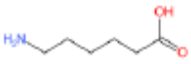
CAS: 96-24-2
Dataset id:349 (Test Set)
SMILES: OCC(O)CCl
Similarity: 0.824
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 57



Compound #4

CAS: 111-46-6
Dataset id:240 (Training Set)
SMILES: OCCOCCO
Similarity: 0.81
Experimental value : Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #5

CAS: 60-32-2
Dataset id:47 (Training Set)
SMILES: O=C(O)CCCCCN
Similarity: 0.805
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #6

CAS: 556-52-5
Dataset id:351 (Training Set)
SMILES: OCC1OC1
Similarity: 0.803
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 105

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3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	Global AD Index AD index = 0.838 Explanation: The predicted compound is into the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.851 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.682 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

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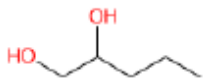
1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Oral Carcinogenic class: Carcinogen
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

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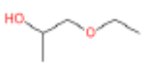
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

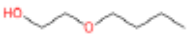
Compound #1

CAS: 57-55-6
Dataset id:661 (Training Set)
SMILES: OCC(O)C
Similarity: 0.905
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #2

CAS: 1569-02-4
Dataset id:663 (Training Set)
SMILES: OC(C)COCC
Similarity: 0.869
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

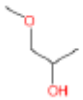


Compound #3

CAS: 111-76-2
Dataset id:509 (Training Set)
SMILES: OCCOCCCC
Similarity: 0.867
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 71-36-3
Dataset id:362 (Training Set)
SMILES: OCCCC
Similarity: 0.865
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #5

CAS: 107-98-2
Dataset id:664 (Training Set)
SMILES: OC(C)COC
Similarity: 0.857
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 78-92-2
Dataset id:363 (Training Set)
SMILES: OC(C)CC
Similarity: 0.855
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

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3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
✔	Similar molecules with known experimental value Similarity index = 0.886 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

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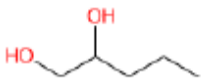
1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is NON-Carcinogen, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: OCC(O)CCC
Experimental value: -
Predicted Inhalation Carcinogenic class: NON-Carcinogen
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

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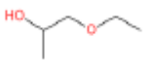
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

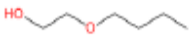
Compound #1

CAS: 57-55-6
Dataset id:650 (Test Set)
SMILES: OCC(O)C
Similarity: 0.905
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #2

CAS: 1569-02-4
Dataset id:652 (Training Set)
SMILES: OC(C)COCC
Similarity: 0.869
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



Compound #3

CAS: 111-76-2
Dataset id:482 (Training Set)
SMILES: OCCOCCCC
Similarity: 0.867
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 71-36-3
Dataset id:314 (Training Set)
SMILES: OCCCC
Similarity: 0.865
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 107-98-2
Dataset id:653 (Training Set)
SMILES: OC(C)COC
Similarity: 0.857
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 78-92-2
Dataset id:316 (Training Set)
SMILES: OC(C)CC
Similarity: 0.855
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

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3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	Global AD Index AD index = 0.941 Explanation: The predicted compound is into the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.886 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

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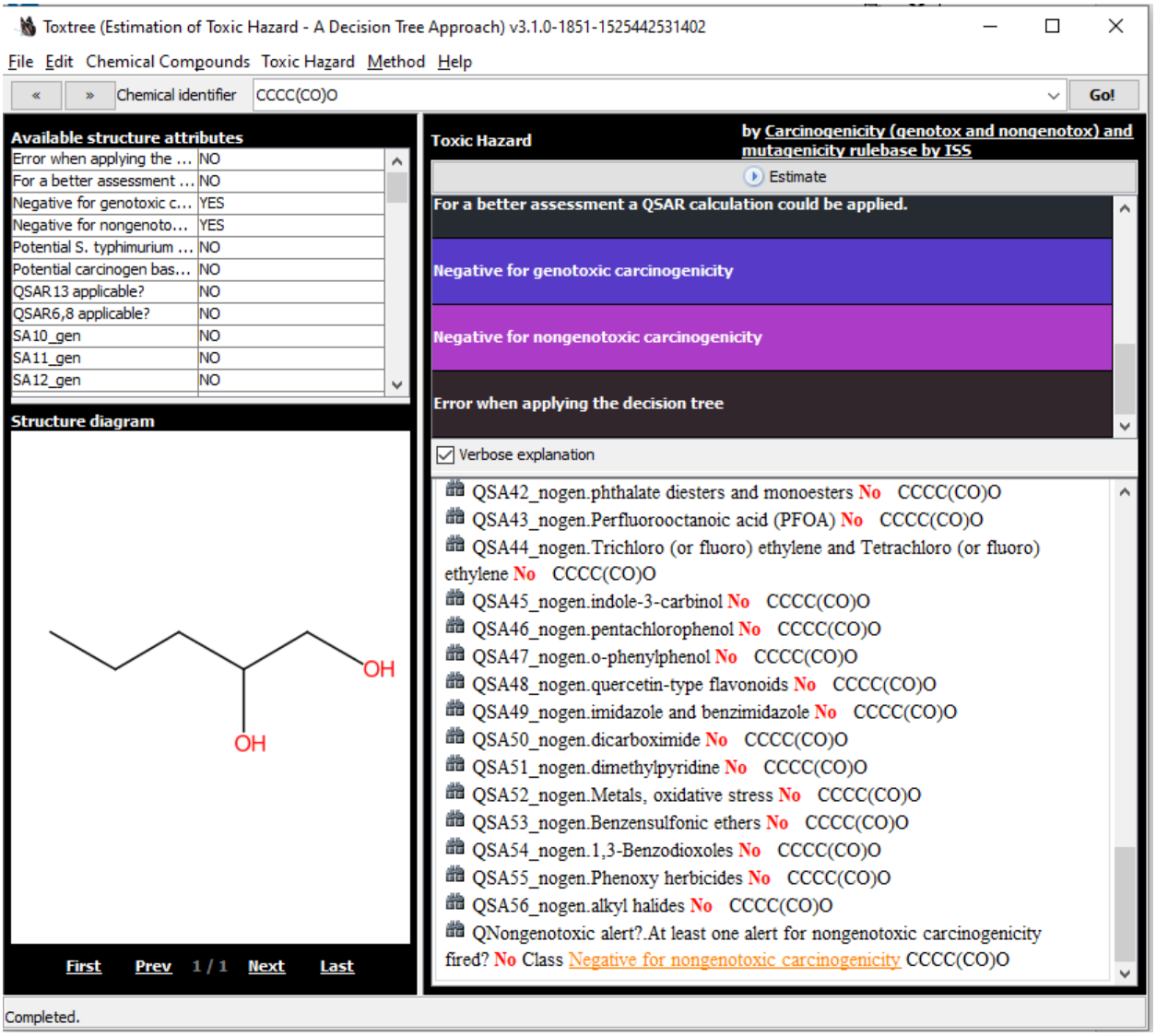
APPENDIX E: Toxtree Carcinogenicity Results for Pentylene Glycol (CAS #5343-92-0)



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APPENDIX F: Danish QSAR Carcinogenicity Results for Pentylene Glycol (CAS #5343-92-0)

Carcinogenicity

	E Ultra	Leadscope
FDA RCA Cancer Male Rat	POS_OUT	INC_OUT
FDA RCA Cancer Female Rat	NEG_IN	NEG_IN
FDA RCA Cancer Rat	NEG_IN	INC_OUT
FDA RCA Cancer Male Mouse	NEG_IN	NEG_OUT
FDA RCA Cancer Female Mouse	NEG_IN	NEG_OUT
FDA RCA Cancer Mouse	NEG_IN	NEG_OUT
FDA RCA Cancer Rodent	NEG_IN	INC_OUT

Commercial models from CASE Ultra and Leadscope

FDA RCA: Data from US Food and Drug Administration as part of Research Cooperation Agreement

Carcinogenicity (genotox and nongenotox) alerts by ISS, alerts in:	
- parent only	No alert found
Oncologic Primary Classification, alerts in:	
- parent only	Not classified

OECD QSAR Toolbox v.4.2 profilers

Profiler predictions are supporting information to be used together with the relevant QSAR predictions

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Liver Specific Cancer in Rat or Mouse		NEG_IN	NEG_IN	NEG_OUT	NEG_IN

DTU-developed models

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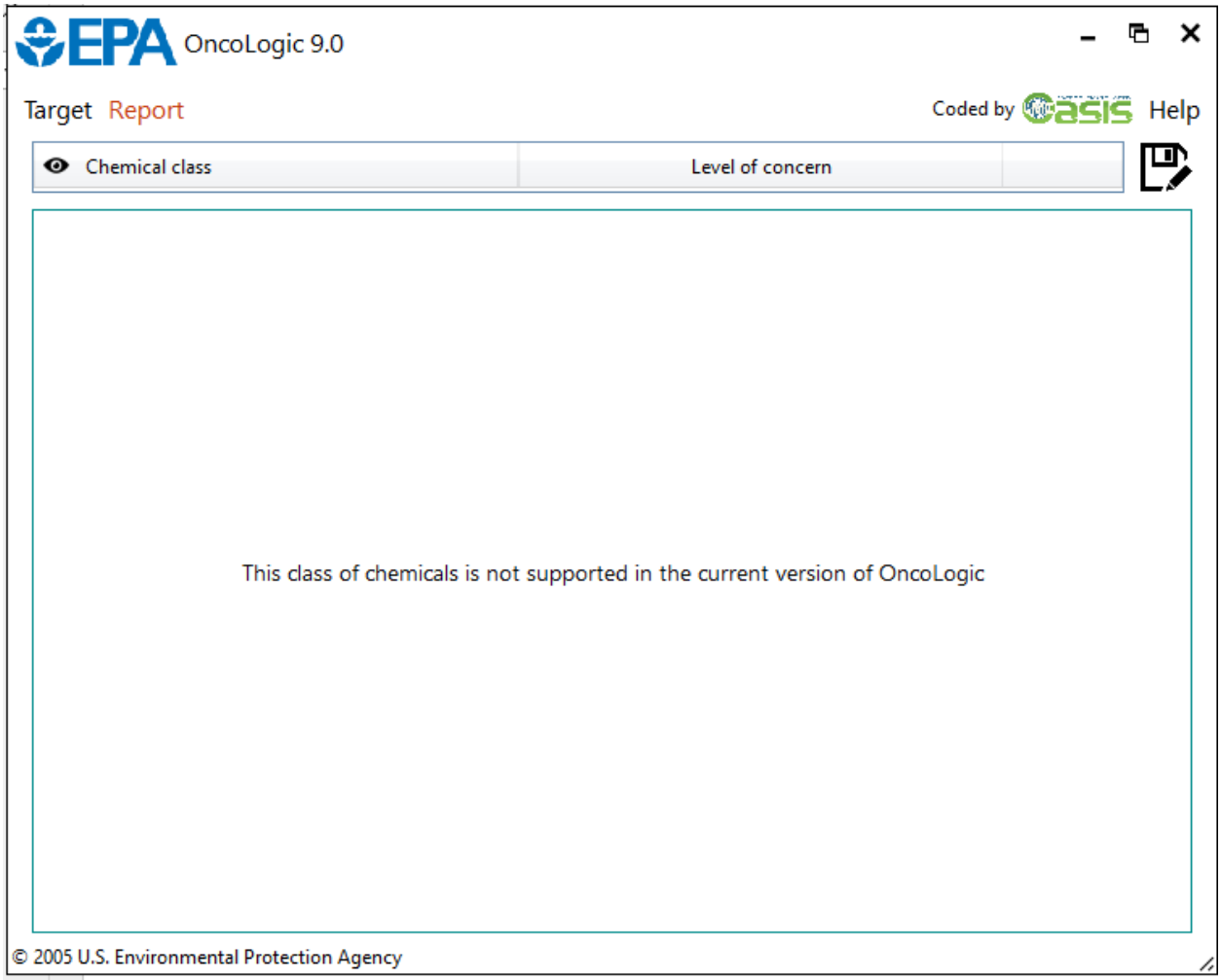
APPENDIX G: OncoLogic Carcinogenicity Results for Pentylene Glycol (CAS #5343-92-0)



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OncoLogic Justification Report

SUMMARY :

CODE NUMBER : 5343920

SUBSTANCE ID :

JUSTIFICATION:

Aliphatic Alcohols*

Aliphatic alcohols (R-OH) may be loosely divided into (a) high M.W.alcohols (C > 20), (b) medium size alcohols (C = 6 to 20), and (c) low M.W. alcohols (C < 6). In general, high M.W. aliphatic alcohols have low potential to be significant carcinogens. A number of medium size alcohols (e.g., CF3(CF2)6CH2OH; 2-ethylhexanol) that can be oxidized to metabolically persistent aliphatic carboxylic acids (e.g., perfluorinated fatty acid like perfluoroooctanoic; ω – 1 branched fatty acids like 2-ethylhexanoic acid) are potential nongenotoxic carcinongens. Most of these are medium sized with the most potent ones peaking around 7 – 9 carbons. Low M.W. alcohols, (especially methanol and ethanol) are of carcinogenic concern because of possible oxidation to reactive aldehydes. The concern for carcinogenic risk is especially higher in individuals who are genetically deficient in aldehyde dehydrogenase which detoxifies aldehydes to carboxylic acids. A number of low M.W. tertiary alcohols (e.g., t-butyl, t-amyl) have been shown to induce kidney tumors in male rats by a mechanism (alpha-2-mu nephropathy) not relevant to humans. In addition, low M.W. alcohols with

(i) terminal double bond or Cl/Br/I,
(ii) α,β-unsaturation,
(iii) monosubstitution with Cl/Br/I at α-carbon are of concern as potential genotoxic carcinogens.

---

*This is only a brief summary of the structure activity relationships (SAR) knowledge of this class. A more detailed decision logic will be developed in future version of OncoLogic. If the compound of your interest has been tested in any short-term predictive tests, the results of the tests should be entered into OncoLogic's Functional Arm to give an evaluation of carcinogenic potential based on short-term predictive tests.

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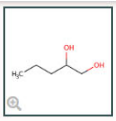
APPENDIX H: ToxCast Model Results for Pentylene Glycol (CAS #5343-92-0)



1,2-Pentanediol

5343-92-0 | DTXSID10863522

Searched by DTXSID10863522

Bioactivity - ToxCast: Models

EXPORT

ToxCast Model Predictions

Model	Receptor	Agonist	Antagonist	Binding
COMPARA (Consensus)	Androgen	0.00	0.00	0
CERAPP Potency Level (From Literature)	Estrogen	Inactive	Inactive	Inactive
CERAPP Potency Level (Consensus)	Estrogen	0.00	0.00	0

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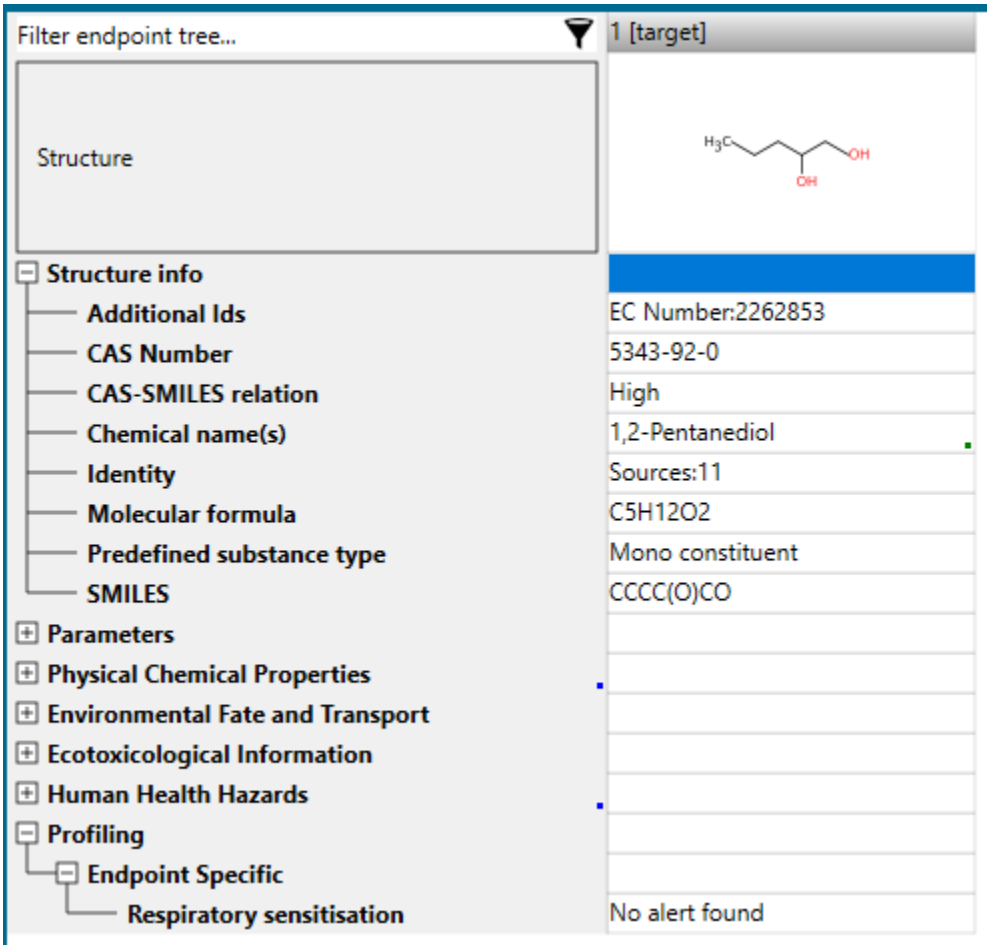
APPENDIX I: OECD Toolbox Respiratory Sensitization Results for Pentylene Glycol (CAS #5343-92-0)



Filter endpoint tree...	1 [target]
Structure	
Structure info	
Additional Ids	EC Number:2262853
CAS Number	5343-92-0
CAS-SMILES relation	High
Chemical name(s)	1,2-Pentanediol
Identity	Sources:11
Molecular formula	C5H12O2
Predefined substance type	Mono constituent
SMILES	CCCC(O)CO
Parameters	
Physical Chemical Properties	
Environmental Fate and Transport	
Ecotoxicological Information	
Human Health Hazards	
Profiling	
Endpoint Specific	
Respiratory sensitisation	No alert found

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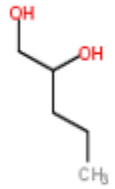
APPENDIX J: ECOSAR Modeling Results for Pentylene Glycol (CAS #5343-92-0)

Organic Module Report

Results of Organic Module Evaluation

CAS	Name	SMILES
5343920		OC(CCC)CO

Structure



Details	
Mol Wt	104.15
Selected LogKow	
Selected Water Solubility (mg/L)	
Selected Melting Point (°C)	
Estimated LogKow	0.2
Estimated Water Solubility (mg/L)	29149.86
Measured LogKow	
Measured Water Solubility (mg/L)	
Measured Melting Point (°C)	104

Class Results:	

Neutral Organics

Organism	Duration	End Point	Concentration (mg/L)	Max Log Kow	Flags
Fish	96h	LC50	3.54E03	5	
Daphnid	48h	LC50	1.70E03	5	
Green Algae	96h	EC50	6.37E02	6.4	
Fish		ChV	2.84E02	8	
Daphnid		ChV	1.04E02	8	
Green Algae		ChV	1.15E02	8	
Fish (SW)	96h	LC50	4.41E03	5	
Mysid	96h	LC50	1.11E04	5	

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Class Results:	

Organism	Duration	End Point	Concentration (mg/L)	Max Log Kow	Flags
Fish (SW)		ChV	1.59E02	8	
Mysid (SW)		ChV	1.63E03	8	
Earthworm	14d	LC50	2.78E02	6	

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APPENDIX K: EPI Suite™ Modeling Results for Pentylene glycol (CAS #5343-92-0)

(Estimated values included in the GreenScreen® are highlighted and bolded)

CAS Number: 005343-92-0
SMILES : OC(CCC)CO
CHEM : Pentane-1,2-diol
MOL FOR: C5 H12 O2
MOL WT : 104.15
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): 0.06
Boiling Point (deg C) : 206.00
Melting Point (deg C) : 104.00
Vapor Pressure (mm Hg) : 0.144
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = 0.20

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 197.05 (Adapted Stein & Brown method)
Melting Pt (deg C): -9.51 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.00535 (Modified Grain method)
VP (Pa, 25 deg C) : 0.714 (Modified Grain method)
MP (exp database): 104 deg C
BP (exp database): 206 deg C
VP (exp database): 1.44E-01 mm Hg (1.92E+001 Pa) at 47 deg C
Subcooled liquid VP: 0.87 mm Hg (47 deg C, user-entered VP)
: 116 Pa (47 deg C, user-entered VP)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 3.974e+004
log Kow used: 0.06 (user entered)
melt pt used: 104.00 deg C

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1e+006 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 3.06E-007 atm-m3/mole (3.10E-002 Pa-m3/mole)
Group Method: 2.62E-010 atm-m3/mole (2.66E-005 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered

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Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.966E-007 atm-m3/mole (5.031E-002 Pa-m3/mole)
VP: 0.144 mm Hg (source: User-Entered)
WS: 3.97E+004 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 0.06 (user entered)
Log Kaw used: -4.903 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 4.963
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 1.0154
Biowin2 (Non-Linear Model) : 0.9774
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.2890 (days-weeks)
Biowin4 (Primary Survey Model) : 3.9564 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.7136
Biowin6 (MITI Non-Linear Model): 0.8733
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.9342
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): 116 Pa (0.87 mm Hg)
Log Koa (Koawin est): 4.963
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 2.59E-008
Octanol/air (Koa) model: 2.25E-008
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 9.34E-007
Mackay model : 2.07E-006
Octanol/air (Koa) model: 1.8E-006

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 17.3026 E-12 cm3/molecule-sec
Half-Life = 0.618 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 7.418 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
1.5E-006 (Junge-Pankow, Mackay avg)
1.8E-006 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

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Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 1 L/kg (MCI method)
Log Koc: 0.000 (MCI method)
Koc : 1.366 L/kg (Kow method)
Log Koc: 0.135 (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 = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.7824 days (HL = 0.01651 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.026 (BCF = 0.9415)
Log BAF Arnot-Gobas method (upper trophic) = -0.026 (BAF = 0.9415)
log Kow used: 0.06 (user entered)

Volatilization from Water:
Henry LC: 3.06E-007 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 1954 hours (81.4 days)
Half-Life from Model Lake : 2.14E+004 hours (891.6 days)

Removal In Wastewater Treatment:
Total removal: 1.87 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.76 percent
Total to Air: 0.02 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	**2.1**	**14.8**	**1000**
Water	**40.8**	**208**	**1000**
Soil	**57**	**416**	**1000**
Sediment	**0.0722**	**1.87e+003**	**0**

Persistence Time: 256 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.1	14.8	1000
Water	40.8	208	1000
water	(40.8)		
biota	(2.34e-006)		
suspended sediment	(6.12e-005)		
Soil	57	416	1000
Sediment	0.0722	1.87e+003	0

Persistence Time: 256 hr

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Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.11	14.8	1000
Water	41.3	208	1000
water	(41.3)		
biota	(2.37e-006)		
suspended sediment	(2.92e-005)		
Soil	56.5	416	1000
Sediment	0.0722	1.87e+003	0

Persistence Time: 255 hr

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APPENDIX L: Change in Benchmark Score

Table 5 provides a summary of changes to the GreenScreen® Benchmark™ for pentylene glycol. The original GreenScreen® assessment was performed in 2024 under version 1.4 criteria and ToxServices assigned a Benchmark 2 (BM-2) score.

Table 5: Change in GreenScreen® Benchmark™ for Pentylene glycol

Date	GreenScreen® Benchmark™	GreenScreen® Version	Comment
February 22, 2024	BM-2	v. 1.4	Original GreenScreen® assessment.
March 18, 2024	BM-2	v. 1.4	No change in BM score or endpoint scores. Improved clarity mainly in the persistence section in response to the comments from WA Department of Ecology.

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Licensed GreenScreen® Profilers

Pentylene Glycol GreenScreen® Evaluation Prepared by:

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Toxicologist
ToxServices LLC

Pentylene Glycol GreenScreen® Evaluation QC'd by:

SIGNATURE BLOCK

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ToxServices LLC