Method Version: GreenScreen® Version 1.2

Verified or Non-Verified: VERIFIED

Date of Verification:	**October 22, 2013**
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GreenScreen® Verification Performed By:	Clean Production Action
	Date: October 22, 2013
	Verification Review Plan Prepared By: Dr. Eric Rosenblum
Verified GreenScreen® Prepared by Licensed Profiler:	Organization: ToxServices LLC
	Date: October 15, 2013

bis(2-Hydroxyethyl) Terephthalate (CAS# 959-26-2) GreenScreen® Assessment

Prepared for:

Clean Production Action

Date:

October 15, 2013 (Verified)

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GreenScreen® Executive Summary for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

bis(2-Hydroxyethyl) terephthalate is a chemical that functions as a reactant in the production of polyethylene terephthalate plastics.

bis(2-Hydroxyethyl) terephthalate was assigned a GreenScreen® Benchmark Score of U ("Unspecified") as there are insufficient data to determine a majority of the hazard rankings for this chemical. Data gaps (DG) exist for Carcinogenicity (C), Reproductive Toxicity (R), Developmental Toxicity (D), Endocrine Activity (E), Acute Toxicity (AT), Systemic Toxicity (single and repeat dose) (ST), Neurotoxicity (single and repeat dose) (N), Skin Sensitization (SnS), Respiratory Sensitization (SnR), Skin Irritation (IrS), Eye Irritation (IrE), Reactivity (Rx), and Flammability (F). The data gaps for bis(2-hydroxyethyl) terephthalate do not meet the minimum data requirements for a Benchmark Score of 2 and the available data do not suggest a high enough hazard for a Benchmark Score of 1 as detailed in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis). In a worst-case scenario, if Bis(2-hydroxyethyl) terephthalate were assigned a High score for Carcinogenicity (C), Reproductive Toxicity (R), Developmental Toxicity (D), or Endocrine Activity (E), it would be categorized as a Benchmark 1 Chemical.

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

GreenScreen® Hazard Ratings for bis(2-Hydroxyethyl) Terephthalate

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

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

GreenScreen® Assessment for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

GreenScreen® Version 1.2 Assessment

Chemical Name: bis(2-Hydroxyethyl) terephthalate

CAS Number: 959-26-2

GreenScreen® Assessment Prepared By:
Name: Zachariah Guerrette, Ph.D.

Title: Toxicologist
Organization: ToxServices LLC
Date: April 8, 2013; October 7, 2013 (Revision #1)

Quality Control Performed By:
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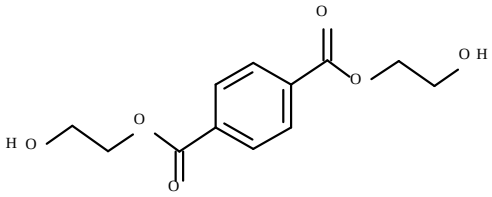
Title: Managing Director and Chief Toxicologist
Organization: ToxServices LLC
Date: April 8, 2013; October 15, 2013 (Revision #1)

Confirm application of the *de minimus* rule[1]: not applicable; bis(2-hydroxyethyl) terephthalate is not a mixture.

Chemical Structure(s):

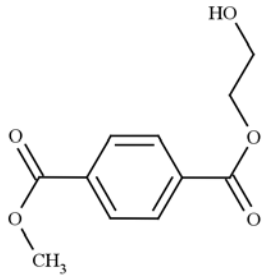


bis(2-Hydroxyethyl) terephthalate (CAS #959-26-2)

Also called: Bis(2-hydroxyethyl) ester 1,4-benzenedicarboxylic acid; Bis(ethylene glycol) terephthalate; Bis(hydroxyethyl) terephthalate; Bis(beta-hydroxyethyl) terephthalate; Bis(2-hydroxyethyl) ester terephthalic acid; BEHT (ChemIDplus 2013)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Data gaps exist for the majority of health effect endpoints. In order to address these data gaps, the use of a chemical surrogate was considered. No chemical surrogates were identified using the U.S. EPA's Analog Identification Methodology (AIM; http://aim.epa.gov/) software. The Structure Similarity Search function in ChemIDplus identified 1,4-Benzenedicarboxylic acid, 1-(2-hydroxyethyl) 4-methyl ester (CAS #3645-00-9) as having 82.39% structural similarity with bis(2-hydroxyethyl) terephthalate. However, a literature search identified insufficient data for 1,4-benzenedicarboxylic acid, 1-(2-hydroxyethyl) 4-methyl ester to address the data gaps for bis(2-hydroxyethyl) terephthalate. Therefore, no chemical surrogate data were used.

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



1,4-Benzenedicarboxylic acid, 1-(2-hydroxyethyl) 4-methyl ester (CAS# 3645-00-9)

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

Identify Applications/Functional Uses:
1. Production of polyethylene terephthalate (PET) plastics (HSDB 2003)

GreenScreen® Summary Rating for bis(2-Hydroxyethyl) Terephthalate[3]: bis(2-Hydroxyethyl) terephthalate was assigned a GreenScreen® Benchmark Score of U ("Unspecified") as there are insufficient data to determine a majority of the hazard rankings for this chemical. Data gaps (DG) exist for Carcinogenicity (C), Reproductive Toxicity (R), Developmental Toxicity (D), Endocrine Activity (E), Acute Toxicity (AT), Systemic Toxicity (single and repeat dose) (ST), Neurotoxicity (single and repeat dose) (N), Skin Sensitization (SnS), Respiratory Sensitization (SnR), Skin Irritation (IrS), Eye Irritation (IrE), Reactivity (Rx), and Flammability (F). The data gaps for bis(2-hydroxyethyl) terephthalate do not meet the minimum data requirements for a Benchmark Score of 2 and the available data do not suggest a high enough hazard for a Benchmark Score of 1 as detailed in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis). In a worst-case scenario, if Bis(2-hydroxyethyl) terephthalate were assigned a High score for Carcinogenicity (C), Reproductive Toxicity (R), Developmental Toxicity (D), or Endocrine Activity (E), it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Ratings for bis(2-Hydroxyethyl) Terephthalate

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

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

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

[3] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

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

Functional Use	Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	List Translator Results
	End of Life	Hydrolysis	Terephthalic Acid	100-21-0	LT-U
	End of Life	Hydrolysis	Ethylene Glycol	107-21-1	LT-1

No transformation products were identified from the literature. Based on the chemical structure, hydrolysis reactions involving the ester functional groups are likely to occur, resulting in the formation of terephthalic acid (CAS #100-21-0) and ethylene glycol (CAS 107-21-1). Ethylene glycol is considered a Benchmark 1 chemical as it is classified as a NTP-OHAaT Category A developmental toxicant - Clear evidence of adverse developmental toxicant effects. However, PET is a hydrolytically stable polymer of bis(2-hydroxyethyl) terephthalate. When used in PET plastics, the ester bond found in bis(2-hydroxyethyl) terephthalate is maintained. Cleavage of this bond is only feasible under neutral pH but requires high temperatures (473-573°K) and high pressure (1-4 MPa) (Carta et al. 2003). The Benchmark score of U is therefore appropriate for bis(2-hydroxyethyl) terephthalate even though ethylene glycol has a Benchmark Score of 1.

Introduction

bis(2-Hydroxyethyl) terephthalate is formed during the synthesis of polyethylene terephthalate (PET) plastics (HSDB 2003). It is generated via esterification of terephthalic acid and is subsequently polymerized via a transesterification reaction to form PET. Antimony oxide is used to catalyze the transesterification reaction. ToxServices assessed bis(2-hydroxyethyl) terephthalate against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.37 (GreenScreen Hazard Assessment)(ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2013) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b) and these should be checked separately in conjunction with running the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for bis(2-hydroxyethyl) terephthalate can be found in Appendix C and a summary of the results can be found below:

[4] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.
[5] The assessment of transformation products depends on the Benchmark Score of the parent chemical (see CPA Guidance 2013).

bis(2-Hydroxyethyl) terephthalate does not have any high or medium hazards for health or ecotoxicity identified in Pharos. bis(2-Hydroxyethyl) Terephthalate is not listed in the U.S. DOT lists (U.S. DOT 2008a,b).

PhysioChemical Properties of bis(2-Hydroxyethyl) terephthalate

bis(2-Hydroxyethyl) terephthalate is an organic chemical with chemical formula $C_{12}H_{14}O_6$ and a molecular weight of 254.24 g/mol. It is a solid at 25 °C with low volatility based on an estimated vapor pressure of 1.11E-07 mm Hg at 25°C. It is estimated to be soluble in water up to 17,600 mg/L at 25°C and it has an estimated log K_{OW} value of 0.12. It is not expected to bioaccumulate in biota due to its low lipophilicity.

Table 1: Physical and Chemical Properties of bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

Property	Value	Reference
Molecular formula	$C_{12}H_{14}O_6$	ChemIDplus 2013
SMILES Notation	c1(C(OCCO)=O)ccc(C(OCCO)=O)cc1	ChemIDplus 2013
Molecular weight	254.24 g/mol	HSDB 2003
Physical state	Solid	Sigma-Aldrich 2012
Appearance	Not identified	
Melting point	106-109°C	Sigma-Aldrich 2012
Vapor pressure	1.11 x 10^{-07} mm Hg at 25°C (estimated)	ChemIDplus 2013
Water solubility	17,600 mg/L at 25°C (estimated)	ChemIDplus 2013
Dissociation constant	Not identified	
Density/specific gravity	1.316 g/cm^3 (estimated)	ChemSpider 2013
Partition coefficient	Log K_{OW} = 0.12 (estimated)	ChemIDplus 2013

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for carcinogenicity based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Mutagenicity/Genotoxicity (M) Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a data gap (DG) for mutagenicity/genotoxicity based on the lack of data identified for this endpoint. Although negative results were obtained in an Ames and micronucleus assays, insufficient detail was available from the article abstract to judge the quality of the assays and the significance of results obtained from them. GreenScreen® criteria

requires that there are no structural alerts and that negative data from a chromosome aberration assay and a gene mutation assay are available for a compound to be assigned a score of Low for mutagenicity/genotoxicity (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- Bach et al. 2013
    - Polyethylene terephthalate (PET) bottles containing water were stored at 40°C, 50°C, or 60°C and extracts in the water were analyzed. bis(2-Hydroxyethyl) terephthalate, an intermediate monomer in the production of PET plastic, was detected in PET-bottled water. PET-bottled water extracts containing bis(2-hydroxyethyl) terephthalate produced negative results in the Ames assay and micronucleus assay performed in a human cell line (no further details available).
- No additional data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Reproductive Toxicity (R) Score (H, M, or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for reproductive toxicity based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for developmental toxicity based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Endocrine Activity (E) Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for endocrine disruption based on the lack of data identified for this endpoint. Although negative results were obtained in estrogenic and anti-androgenic activity assays, insufficient detail was available from the article abstract to judge the quality of the assays and the significance of results obtained from them. GreenScreen® criteria require that negative data from endocrine activity studies are available for a compound to be assigned a score of Low for endocrine activity (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Bach et al. 2013 –
    - Polyethylene terephthalate (PET) bottles containing water were stored at 40°C, 50°C, or

60°C and extracts in the water were analyzed. bis(2-Hydroxyethyl) terephthalate, an intermediate monomer in the production of PET plastic, was detected in PET-bottled water. PET-bottled water extracts containing bis(2-hydroxyethyl) terephthalate produced negative results in transcriptional-reporter gene assays for estrogenic and anti-androgenic activity (no further details available).

- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

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

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

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

bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for acute toxicity based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)

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

bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for systemic toxicity (single dose) based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

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

bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for systemic toxicity (repeated dose) based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Neurotoxicity (N)

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

bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for neurotoxicity (single dose) based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Group II* Score (repeated dose)**(H, M, or L):** DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for neurotoxicity (repeated dose) based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Skin Sensitization (SnS) Group II* Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for skin sensitization based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Respiratory Sensitization (SnR) Group II* Score (H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for respiratory sensitization based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for skin irritation/corrosivity based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Ecotoxicity (Ecotox)

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

bis(2-Hydroxyethyl) terephthalate was assigned a score of Low for acute aquatic toxicity based on the most conservative estimated acute aquatic L/EC50 value being 618.23 mg/L. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when the most conservative acute aquatic toxicity value is >100 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No measured data are available for the acute aquatic toxicity of bis(2-hydroxyethyl) terephthalate or its surrogate. Estimated values were generated with ECOSAR v.1.11 (U.S. EPA 2012a) and the complete ECOSAR output is available in Appendix D.
  - Estimated water solubility = 17,610 mg/L
  - Ester class
    - 96-hour LC_{50} (fish) = 424.49 mg/L
    - 48-hour LC_{50} (daphnid) = 1,078.88 mg/L
    - 96-hour EC_{50} (green algae) = 618.23 mg/L
  - Neutral Organics class
    - 96-hour LC_{50} (fish) = 10,141.90 mg/L
    - 48-hour LC_{50} (daphnid) = 4,842.03 mg/L
    - 96-hour EC_{50} (green algae) = 1,761.25 mg/L

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

bis(2-Hydroxyethyl) terephthalate was assigned a score of Low for chronic aquatic toxicity based on the most conservative chronic aquatic toxicity value being 47.36 mg/L. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when the most conservative chronic aquatic toxicity value is >10 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No measured data are available for the chronic aquatic toxicity of bis(2-hydroxyethyl) terephthalate or its surrogate. Estimated values were generated with ECOSAR v.1.11 (U.S. EPA 2012a) and the complete ECOSAR output is available in Appendix D.
  - Estimated water solubility = 17,610 mg/L
  - Esters class
    - Chronic value (fish) = 47.36 mg/L
    - Chronic value (daphnid) = 1,265.86 mg/L
    - Chronic value (green algae) = 86.14 mg/L
  - Neutral Organics class
    - Chronic value (fish) = 808.00 mg/L
    - Chronic value (daphnid) = 291.47 mg/L
    - Chronic value (green algae) = 313.51 mg/L

Environmental Fate (Fate)

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

bis(2-Hydroxyethyl) terephthalate was assigned a score of Moderate for persistence based on it having an estimated half-life in soil of 30 days. GreenScreen® criteria classify chemicals as a Moderate hazard for persistence when soil half-lives are between 16 and 60 days (CPA 2012a).

Authoritative and Screening Lists

- *Authoritative:* not listed in any authoritative lists
- *Screening:* not listed in any screening lists

- No measured environmental persistence data are available for bis(2-hydroxyethyl) terephthalate or its surrogate. Estimated values for persistence were generated with EPI Suite v4.11 (U.S. EPA 2012b) and the complete EPI Suite output is available in Appendix E.
  - Biowin models of biodegradation predict that bis(2-hydroxyethyl) terephthalate is readily biodegradable.
  - Biowin models of biodegradation also suggest that the primary degradation of bis(2-hydroxyethyl) terephthalate will occur in days (Biowin4) and the ultimate degradation to water and carbon dioxide will occur over a period of weeks (Biowin3).
  - In a model of wastewater treatment, 1.85% of bis(2-hydroxyethyl) terephthalate is estimated to be removed from wastewater, with 0.09% being removed via biodegradation and the remaining 1.76% being through sludge adsorption.
  - Fugacity modeling predicts 69.4% of bis(2-hydroxyethyl) terephthalate will partition to soil with a half-life of 30 days and 30.6% will partition to water with a half-life of 15 days. Based on the modeled data, bis(2-hydroxyethyl) terephthalate is expected to persist in the environment as it has half-lives of 30 days in the major environmental compartments.
- Although the BIOWIN model predicts that bis(2-hydroxyethyl) terephthalate is going to be readily biodegradable, no experimental data is available to demonstrate the biodegradation. The results of the fugacity models were used as the basis for the moderate score for persistence in order to be more conservative.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *vL*

bis(2-Hydroxyethyl) terephthalate was assigned a score of Very Low for bioaccumulation based on an estimated log K_{OW} value of 0.12 and an estimated BCF value of 3.162. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when log K_{OW} values are $\leq$ 4 and when BCF values are < 100 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed in any authoritative lists
  - *Screening:* not listed in any screening lists
- No measured environmental persistence data are available for bis(2-hydroxyethyl) terephthalate or its surrogate. Estimated values were generated with EPI Suite v4.11 (U.S. EPA 2012b) and the complete EPI Suite output is available in Appendix E.
  - An estimated log K_{OW} = 0.12 suggests a very low potential to bioaccumulate in aquatic biota.
  - An estimated bioconcentration factor (BCF) = 3.162 suggests a very low potential to bioaccumulate in aquatic biota.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for reactivity based on the lack of data available for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

Flammability (F) Score (vH, H, M or L): DG
bis(2-Hydroxyethyl) terephthalate was assigned a Data Gap for flammability based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* not listed in any authoritative lists
    - *Screening:* not listed in any screening lists
- No data were identified for this endpoint for bis(2-hydroxyethyl) terephthalate or its surrogate.

References

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APPENDIX A: Hazard Benchmark Acronyms (in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(Cr) Corrosion/ Irritation (Skin/ Eye)

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GreenScreen™ Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	bis(2-Hydroxyethyl) Terephthalate	959-26-2	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	DG	L	L	M	vL	DG	DG

Table 3a: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen™ Benchmark Score
bis(2-Hydroxyethyl) Terephthalate	3

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

Table 6

Chemical Name	Final GreenScreen™ Benchmark Score
bis(2-Hydroxyethyl) Terephthalate	U

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

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2												
3	No	No	Yes	Yes	No	No	No	Yes	Yes	No		U
4												

APPENDIX C: Pharos Output for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

BIS(2-HYDROXYETHYL) TEREPHTHALATE

CAS RN: 959-26-2

Synonyms: 1,4-BENZENEDICARBOXYLIC ACID, BIS(2-HYDROXYETHYL) ESTER

Direct Chemical and Compound Hazard Quickscreen — Detailed Hazard Listings

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

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

Life Cycle Research

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

Description: "ESSENTIALLY 100% AS CAPTIVE CHEM INT FOR POLYETHYLENE TEREPHTHALATE" (Hazardous Substances Data Bank)

View Products Containing This Chemical

Compound Groups

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

Tags for this chemical

There are no tags for this chemical yet.

Add a New Tag

Sources

Hazardous Substances Databank (HSDB) (NHIS)

CAS Variants

APPENDIX D: ECOSAR Modeling Results for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

ECOSAR Version 1.11 Results Page

SMILES : O=C(OCCO)c(ccc(c1)C(=O)OCCO)c1
CHEM : 1,4-Benzenedicarboxylic acid, bis(2-hydroxyethyl) ester
CAS Num: 000959-26-2
ChemID1:
MOL FOR: C12 H14 O6
MOL WT : 254.24
Log Kow: 0.122 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 1.761E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 0.122 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 1.761E+004 (mg/L, EPISuite WSKowwin v1.43 Estimate)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Esters

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Esters	: Fish	96-hr	LC50	424.488
Esters	: Daphnid	48-hr	LC50	1078.881
Esters	: Green Algae	96-hr	EC50	618.233
Esters	: Fish		ChV	47.359
Esters	: Daphnid		ChV	1265.860
Esters	: Green Algae		ChV	86.141
Esters	: Fish (SW)	96-hr	LC50	724.451
Esters	: Mysid	96-hr	LC50	1797.279

Esters	: Fish (SW)		ChV	74.060
Esters	: Mysid (SW)		ChV	6.07e+006 *
Esters	: Earthworm	14-day	LC50	13359.335

Neutral Organic SAR	: Fish	96-hr	LC50	10141.897
(Baseline Toxicity)	: Daphnid	48-hr	LC50	4842.029
	: Green Algae	96-hr	EC50	1761.251
	: Fish		ChV	807.995
	: Daphnid		ChV	291.466
	: Green Algae		ChV	313.510

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

Class Specific LogKow Cut-Offs

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

Esters:

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

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

APPENDIX E: EPISuite Modeling Results for bis(2-Hydroxyethyl) Terephthalate (CAS #959-26-2)

CAS Number: 959-26-2
SMILES : O=C(OCCO)c(ccc(c1)C(=O)OCCO)c1
CHEM : 1,4-Benzenedicarboxylic acid, bis(2-hydroxyethyl) ester
MOL FOR: C12 H14 O6
MOL WT : 254.24
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = 0.12

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 378.60 (Adapted Stein & Brown method)
Melting Pt (deg C): 77.16 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 1.11E-007 (Modified Grain method)
VP (Pa, 25 deg C) : 1.48E-005 (Modified Grain method)
Subcooled liquid VP: 3.48E-007 mm Hg (25 deg C, Mod-Grain method)
: 4.64E-005 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 1.761e+004
log Kow used: 0.12 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 4.8603e+005 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Esters

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 5.27E-013 atm-m3/mole (5.34E-008 Pa-m3/mole)
Group Method: 1.47E-017 atm-m3/mole (1.49E-012 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.109E-012 atm-m3/mole (2.137E-007 Pa-m3/mole)
VP: 1.11E-007 mm Hg (source: MPBPVP)
WS: 1.76E+004 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 0.12 (KowWin est)
Log Kaw used: -10.667 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 10.787
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 1.2923
Biowin2 (Non-Linear Model) : 0.9999
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.2377 (weeks)
Biowin4 (Primary Survey Model) : 4.1977 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 1.1961
Biowin6 (MITI Non-Linear Model): 0.9864
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 1.1676
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): 4.64E-005 Pa (3.48E-007 mm Hg)
Log Koa (Koawin est): 10.787
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.0647
Octanol/air (Koa) model: 0.015
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.7
Mackay model : 0.838
Octanol/air (Koa) model: 0.546

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 12.1404 E-12 cm3/molecule-sec
Half-Life = 0.881 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 10.572 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.769 (Junge-Pankow, Mackay avg)
0.546 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 10 L/kg (MCI method)
Log Koc: 1.000 (MCI method)

Koc : 1.09 L/kg (Kow method)
Log Koc: 0.037 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Total Kb for pH > 8 at 25 deg C : 3.704E-001 L/mol-sec
Kb Half-Life at pH 8: 21.657 days
Kb Half-Life at pH 7: 216.567 days
(Total Kb applies only to esters, carbmates, alkyl halides)

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) = -3.0610 days (HL = 0.0008689 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.037 (BCF = 0.9185)
Log BAF Arnot-Gobas method (upper trophic) = -0.037 (BAF = 0.9185)
log Kow used: 0.12 (estimated)

Volatilization from Water:
Henry LC: 5.27E-013 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 1.771E+009 hours (7.381E+007 days)
Half-Life from Model Lake : 1.932E+010 hours (8.052E+008 days)

Removal In Wastewater Treatment:
Total removal: 1.85 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.76 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.9e-005	21.1	1000
Water	30.6	360	1000
Soil	69.4	720	1000
Sediment	0.0688	3.24e+003	0

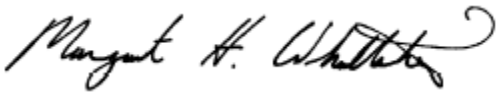
Persistence Time: 640 hr

Authorized Reviewers

bis(2-Hydroxyethyl) Terephthalate GreenScreen® Evaluation Prepared By:

Zachariah Guerrette, Ph.D.
Toxicologist
ToxServices LLC

bis(2-Hydroxyethyl) Terephthalate GreenScreen® Evaluation QC'd By:



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