ACC North American Flame Retardant Alliance

Attached are comments from the American Chemistry Council's North American Flame Retardant Alliance.

American Chemistry Council | North American Flame Retardant Alliance

January 18, 2023

Washington Department of Ecology
300 Desmond Drive SE
Lacey, Washington 98503

Re: Safer Products for Washington – Cycle 1 and evaluating organohalogen flame retardants in plastic casings and enclosures for electronic and electrical equipment

To Whom It May Concern:

The American Chemistry Council's (ACC) North American Flame Retardant Alliance ("NAFRA")[1] is submitting new information to the Washington Department of Ecology ("Department" or "Ecology") relevant to Safer Products for Washington – Cycle 1. The new information is intended to assist the Department in its evaluation of the use of organohalogen flame retardants (OFRs) in plastic casings and enclosures for electronic and electrical equipment.

The attached information includes the following:

- Analysis from Gradient on the Department's criteria for evaluating OFRs and identified alternatives; and,
- Certified GreenScreen® Risk Assessment for 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy) (CAS RN 25713-60-4).

Gradient is a licensed GreenScreen® profiler and performed the GreenScreen® risk assessment for the OFR also known as Tris(tribromophenoxy)triazine (TTBPT). A score of Benchmark 2 has been assigned for TTBPT as part of the GreenScreen® risk assessment. Last year, NAFRA submitted to the Department a GreenScreen Risk Assessment for another OFR, decabromodiphenyl ethane (CAS RN 84852-53-9),[2] which was also assigned a score of Benchmark 2. The Department's minimum criteria for safer is derived from GreenScreen® Benchmark 2 criteria.[3]

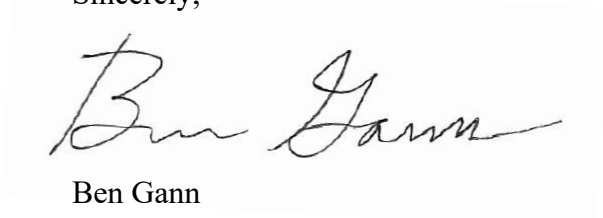
[1] The American Chemistry Council's North American Flame Retardant Alliance represents the leading producers of flame retardants used in wide variety of industrial and consumer applications. NAFRA members represent cutting edge fire-safety chemistry and technology and are dedicated to improving fire safety performance in key product applications. NAFRA members are Albemarle Corporation, ICL Industrial Products, and Lanxess. For more information on NAFRA, visit https://www.americanchemistry.com/industry-groups/north-american-flame-retardant-alliance-nafra.

[2] Gradient. GreenScreen® Assessment for [Decabromodiphenyl ethane; DBDPE (CAS # 84852-53- 9)]; Prepared for: American Chemistry Council: December 2021.

[3] Washington Department of Ecology, Regulatory Determinations Report to the Legislature, Publication 22-04-018, June 2022, p. 289, https://apps.ecology.wa.gov/publications/documents/2204018.pdf

NAFRA appreciates the opportunity to provide additional information as part of Safer Products for Washington – Cycle 1 and the Department's evaluation of OFRs in casings and enclosures of electronic and electrical equipment. Separately, we plan to submit comments to Ecology on the Draft Rule[4] by the February 5 deadline. If you have questions or need clarification on the information provided, please contact me at ben_gann@americanchemistry.com or 202-249-7000.

Sincerely,



Ben Gann
Director, American Chemistry Council
On behalf of the North American Flame Retardant Alliance

[4] Washington Department of Ecology, Safer Products Restrictions and Reporting, December 2022, https://ecology.wa.gov/DOE/files/34/34868dd6-a7ea-4944-814f-010df10dde99.pdf.

Appendix I

January 13, 2023

Mr. Ben Gann
Director, Chemical Products and Technology
American Chemistry Council
700 2nd St, NE
Washington, DC 20002

RE: Washington Department of Ecology Evaluation of Flame Retardant Alternatives

Dear Mr. Gann:

You recently requested that Gradient review the Washington State Department of Ecology's (DOE or Ecology) evaluation of priority halogenated and organophosphate-based flame retardants under the Safer Product for Washington program. Specifically, you requested we evaluate DOE's approach for evaluating the hazards of the flame retardants in question. That evaluation is in part based on the GreenScreen™ method for evaluating specific hazards of chemicals. Gradient is an authorized GreenScreen Profiler.

After examining the DOE approach and reviewing their regulatory determination report[1] (DOE, 2022) we can offer the following observations and opinions:

1. DOE has adopted a hazard evaluation method informally referred to as GreenScreen Plus (note that Ecology does not appear to use this term, at least in written documentation). Essentially, this uses aspects of the GreenScreen method to establish "minimum criteria for safer" but then goes beyond it, particularly for certain chemical classes (in this case halogenated flame retardants) and imposes "additional criteria for safer". While there is nothing in the GreenScreen methodology that specifically prohibits adding other criteria, Gradient does have concerns whether DOE's new approach could undermine the acceptance of GreenScreen. That is, whether chemicals that satisfy the typical use of GreenScreen (*e.g.*, no Benchmark 1 chemicals) will now not meet the Ecology criteria, and therefore be viewed as "bad "chemicals. Note that GreenScreen Benchmark 2 is "use but search for safer substitutes," which implies they are not optimal but also implies that we can or should use them if chemicals with Benchmark 3 or 4 are not suitable for a specific need. Various certification programs (e.g., TCO, GreenScreen Certified) use a prohibition of GreenScreen Benchmark 1 chemicals as their basis for acceptability. DOE creating a new, more stringent categorization could lead to confusion and undermine the assurance provided in the other programs that have adopted the GreenScreen methodology.

2. DOE has assessed the organohalogen flame retardants (HFRs) collectively as an overall class as required by RCW 70A.350.010. Consequently DOE imposed their additional criteria for safer on this group of chemicals and concluded that none of the HFRs they evaluated met their within-class criteria and that as a class, the HFRs are potentially hazardous. However, DOE did not take a similar approach with organophosphorus flame retardants, and reviewed them as individual chemicals using the minimum criteria for safer. A review of the GreenScreen hazard scores for a series of halogenated and organophosphate flame retardants (Table 1) shows that each category contains chemicals with a substantial number of high and very high scores as well as chemicals

[1] Washington Department of Ecology, "Regulatory Determinations Report to the Legislature," June 2022, https://apps.ecology.wa.gov/publications/documents/2204018.pdf.

with a substantial number of low and very low scores.[2] In looking at these GreenScreen hazard determinations, the DOE approach of treating HFRs as a class requiring additional criteria be met and not treating the organophosphate flame retardants similarly appears inconsistent. The result is that a number of lower hazard brominated flame retardants are excluded from consideration while a number of organophosphorus flame retardants with higher hazards are not excluded.

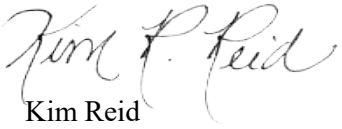
3. DOE has identified resorcinol bis diphenyl phosphate (RDP, CAS 57583-54-7) as one of the acceptable safer organophosphorous flame retardant alternatives. This conclusion was not based on a GreenScreen assessment approach, but rather on a SciVera GHS+™ determination, which concluded it was "yellow" overall, as well as a ChemFORWARD designation of hazard band C, and thus meets the minimum criteria for safer defined by DOE. We do not have the SciVera GHS+ assessment available for review, however, based on a GreenScreen for RDP that Gradient has conducted, although RDP meets DOE's minimum criteria for safer, it would not meet DOE's *additional* criteria for safer using GreenScreen hazard assignments because it scored moderate for carcinogenicity. The use of GHS+ reviews in lieu of GreenScreen evaluations introduces some inconsistency into the evaluation process since, depending on which approach is used, RDP also does not meet the additional criteria for safer defined by DOE.

4. We recently conducted GreenScreen evaluations of two halogenated flame retardants, 2,4,6-tris(2,4,6-tribromophenoxy (CAS 25713-60-4) and decabromodiphenyl ethane (CAS 84852-53-9; results included in Table 1). Both chemicals are scored as GreenScreen Benchmark 2 chemicals, largely due to very high persistence. However, both chemicals have low bioaccumulation potential, low aquatic toxicity and are not carcinogens, mutagens, reproductive or developmental toxicants, or endocrine (CMRDE), thus they would meet the minimum criteria for safer. The fact that they meet the minimum criteria is not consistent with DOE's overall assessment of the HFR class[3]. As indicated in Table 2, the recent GreenScreen assessments of these chemicals suggests they are chemicals of relatively low hazard, comparable if not of lower overall hazard than two of Ecology's identified alternatives. Yet because of Ecology's approach in imposing additional criteria solely on the class of HFRs, these two relatively safer chemicals are prematurely eliminated.

Thank you for the opportunity to provide our perspectives on this matter. Please feel free to contact us if you have any further questions.

Sincerely,

Thomas A. Lewandowski, Ph.D., DABT, ATS
Principal



Kim Reid
Principal Scientist

[2] Note that these hazard scores are provided for illustration only. GreenScreen hazard scores and benchmarks can only be used to make claims about products if accompanied by a full GreenScreen report.

[3] "Studies associate many HFRs with carcinogenicity, mutagenicity, reproductive and developmental toxicity, or endocrine disruption (see hazards of data rich HFRs). In order to confirm that each HFR does not share these hazards, the within-class criteria requires evidence that the chemical is not associated with these endpoints." (see p. 42; DOE, 2022)

Appendix I

Table 1. Comparison of Hazard Summary Tables for Halogenated and Organophosphorous Flame Retardants

Common Name	Acronym	CAS	Benchmark Score	Source	Date	C	M	R	D	E	AT	ST (SE)	ST (RE)	N (SE)	N (RE)	SnS	SnR	IrS	IrE	AA	CA	P	B	F	Total H in Group 1 HH Endpoints
HFRs																									
Decabromodiphenyl ethane	DBDPE	84852-53-9	2	Gradient	2021	*L*	**L**	*M*	*M*	**M**	**L**	**L**	**L**	**L**	*L*	**L**	DG	**L**	**L**	**L**	*L*	*vH*	**L**	**L**	0
1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy)-	TTBPT	25713-60-4	2	Gradient	2022	*L*	*L*	*L*	**L**	*M*	**L**	**L**	**L**	*L*	**L**	**L**	*L*	**L**	**L**	**L**	*L*	*vH*	*L*	**L**	0
DecaBDE		1163-19-5	1	Danish EPA	2016	**M**	**L**	**L**	**H**	**H**	**L**	DG	**M**	DG	*L*	**L**	DG	**L**	**L**	*L*	*L*	**vH**	*H*		2
2,2-Bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	V6	38051-10-4	2	WA DOE[b]	2014	*M*	**L**	**L**	**M**	**M**	**L**	NA	**M**	NA	**L**	**L**	DG	**M**	**M**	**M**	*H*	**vH**	*vL*	*L*	0
Tetrabromobisphenol A	TBBPA	79-94-7	1	WA DOE[b]	2014	**M**	**L**	**L**	**M**	**M**	**L**	NA	*L*	NA	**L**	**L**	DG	**L**	**M**	**vH**	**H**	**H**	**M**	*L*	0
Tetrabromobisphenol A	TBBPA	79-94-7	1	Danish EPA	2016	**M**	**L**	**L**	**M**	**H**	**L**	DG	**L**	**L**	**L**	**L**	DG	**L**	**M**	**vH**	**H**	**H**	**M**		1
2-Ethylhexyltetrabromobenzoate	TBB	183658-27-7	2	WA DOE[b]	2014	*M*	*L*	*M*	*M*	*M*	**L**	NA	*M*	NA	*M*	*M*	DG	*M*	*M*	*L*	*L*	*H*	**H**	*L*	0
Bis(2-ethylhexyl) tetrabromophthalate	TBPH	26040-51-7	2	WA DOE[b]	2014	*M*	**M**	*M*	*M*	*M*	**L**	NA	*M*	NA	*M*	**L**	DG	**M**	**M**	*L*	*L*	*H*	**H**	*L*	0
Hexabromocyclododecane	HBCDD	25637-99-4	1	Danish EPA	2016	*M*	**L**	**M**	**H**	**H**	**L**	DG	**M**	*M*	*M*	**L**	DG	**L**	**L**	**vH**	**vH**	H	**L**		2
OPFRs																									
Tetraphenyl m-phenylene bis(phosphate); resorcinol bis diphenyl phosphate	RDP	57583-54-7	2	Gradient	2019	*M*	**L**	**L**	**L**	*M*	**L**	**L**	**M**	NA	**L**	*L*	DG	**L**	**L**	**L**	*L*	**M**	*H*	**L**	0
Tris(2-chloroisopropyl) phosphate	TCPP	13674-84-5	U[a]	WA DOE[b]	2014	DG	*L*	**M**	**M**	**M**	**L**	NA	*L*	NA	**M**	**L**	DG	**L**	**M**	**H**	*M*	**vH**	**vL**	*L*	0
Tris(2-chloroisopropyl) phosphate	TCPP	13674-84-5	1	Danish EPA	2016	*M*	**L**	**H**	**H**	*M*	**L**	DG	**M**	*M*	**M**	**L**	DG	**L**	**L**	**M**	**M**	**H**	**L**		2
Tris(2-chloroethyl) phosphate	TCEP	115-96-8	1	WA DOE[b]	2014	**H**	**M**	**M**	**M**	*M*	*M*	NA	*M*	**vH**	**M**	**L**	DG	**M**	**M**	**H**	**M**	**M**	**vL**	*L*	1
Tris(1,3-dichloro-2-propyl) phosphate	TDCPP	13674-87-8	1	WA DOE[b]	2014	**H**	**M**	**M**	*M*	**M**	**L**	NA	**M**	NA	**L**	*L*	DG	**M**	**M**	**H**	**H**	*vH*	**L**	*L*	1
Triphenyl phosphate[c]	TPP	115-86-6	2	WA DOE[b]	2014	*M*	**L**	**L**	**L**	**M**	**L**	NA	**H**	NA	**L**	**L**	DG	**L**	**M**	**vH**	**vH**	**L**	**L**	**L**	0
Tricresyl phosphate	TCP	1330-78-5 / 78-30-8	1	WA DOE[b]	2014	*L*	**M**	**H**	**L**	*M*	**vH**	**vH**	*H*	**vH**	**H**	**M**	DG	*L*	*L*	*vH*	*vH*	**vL**	*M*	**L**	1
Isopropylated triphenyl phosphate	IPTPP	68937-41-7	2	WA DOE[b]	2014	*M*	*L*	**M**	**M**	*M*	**L**	NA	*H*	*H*	*M*	*L*	DG	*L*	*M*	*vH*	*vH*	*M*	*H*	*L*	0
Isopropyl phenyl phosphate	IPTPP	68937-41-7	1	Danish EPA	2015	*M*	**L**	**H**	**M**	DG	**L**	DG	**H**	*H*	**H**	**L**	DG	**L**	**L**	**vH**	**vH**	**M**	**vH**		1
9,10-Dihydro-9-oxa-10phosphaphenanthren-10-oxide	DOPO	35948-25-5	2	Danish EPA	2014	*M*	**L**	*L*	*M*	DG	*L*	DG	*L*	DG	*M*	*M*	DG	**L**	**M**	*L*	*M*	*H*	*vL*		0
N,N-bis-(2-hydroxylethyl) aminomethane phosphonic acid diethyl ester		2781-11-5	2	Danish EPA	2015	*M*	**M**	**L**	**L**	DG	**L**	DG	*M*	DG	*M*	*M*	DG	*L*	**L**	**M**	**L**	**H**	**L**		0
Poly(m-phenylene methylphosphonate)		63747-58-0	1	Danish EPA	2014	*L*	*L*	*M*	*M*	*H*	**L**	DG	*M*	DG	*M*	**L**	DG	*L*	*L*	*H*	*H*	*vH*	*H*		1
Poly[phosphonate-co-carbonate]		77226-90-5	3	Danish EPA	2014	*L*	*L*	*L*	*L*	*L*	**L**	*L*	*L*	*L*	*L*	*L*	DG	*L*	*L*	*L*	*L*	*vH*	*L*		0
Triphenyl phosphate	TPHP	115-86-6	1	Danish EPA	2014	**M**	**L**	**L**	**L**	*H*	**L**	DG	**H**	DG	**L**	**L**	DG	**L**	**L**	**vH**	**vH**	**L**	**L**		1
Tricresyl phosphate	TMPP	1330-78-5	1	Danish EPA	2015	**L**	**L**	**H**	**M**	DG	**M**	DG	**H**	DG	**M**	**M**	DG	**L**	**L**	**vH**	**H**	**M**	**H**		1
Bisphenol A bis(diphenyl phosphate)	BPA-BDPP	5945-33-5/ 181028-79-5	2	Danish EPA	2014	*M*	*L*	DG	*L*	DG	**L**	DG	**L**	DG	**L**	**L**	DG	*L*	*L*	**L**	**L**	*H*	*M*		0
Melamine pyrophosphate		15541-60-3	2	Danish EPA	2016	*M*	*M*	*L*	*L*	DG	**L**	DG	*M*	*L*	*L*	*L*	DG	*L*	*L*	**L**	*L*	*H*	*L*		0

Notes:

(a) U = Unspecified due to insufficient data.

(b) GreenScreen assessments are from the IC2 Chemical Hazard Assessment Database.

(c) TPP and EHDPP are OPFRs that meet WA Dept Ecology minimum criteria for Safer.

Appendix I

Table 2. Comparison of Washington Department of Ecology Preferred FR Alternatives to Recently Assessed FRs (Select Endpoints)

Flame Retardant	GreenScreen Endpoints									Minimum Criteria for Safer	Additional Criteria for Safer
	C	M	R	D	E	AA	CA	P	B		
TPP[1]	*M*	**L**	**L**	**L**	**M**	**M**	**vH**	**L**	**L**	Meets	Does Not Meet (M - C)
RDP[2]	*M*	**L**	**L**	**L**	*M*	*L*	*L*	**M**	*H*	Meets	Does Not Meet (M – C)
DBDPE[2]	*L*	**L**	*M*	*M*	**M**	**L**	*L*	*vH*	**L**	Meets	Does Not Meet (vH - P)
TTBPT[2]	*L*	*L*	*L*	**L**	*M*	**L**	*L*	*vH*	*L*	Meets	Does Not Meet (vH - P)

(1) From WA DOE, 2022

(2) From Gradient GreenScreen® assessments. For review and discussion purposes only. GreenScreen benchmarks and hazard scores used in product safety claims are not valid unless accompanied by the associated full GreenScreen asssessment reports.

Report
1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy) (CAS # 25713-60-4)
Certified GreenScreen® Assessment

Prepared for
Sander Kroon
ICL Group
Koningin Wilhelminaplein 30
1062 KR Amsterdam

June 2, 2022

GRADIENT

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GreenScreen® Assessment for 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy) (CAS # 25713-60-4)

Method Version: GreenScreen Version 1.4[1]

Assessment Type:[2] Certified

Chemical Name: 1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy) (CAS # 25713-60-4)

GreenScreen Assessment Prepared By:	**GreenScreen Assessment Quality Control Performed By:**
Name: Ife Bamgbose, M.S.	**Name:** Alexander Alverson
Title: Environmental Scientist	**Title:** Chemist
Organization: Gradient	**Organization:** Gradient
Date: 6/2/2022	**Date:** 6/2/2022
Name: Destiny Mims	**Name:** Charlotte Marsh, M.S., CPPS
Title: Environmental Scientist	**Title:** Toxicologist
Organization: Gradient	**Organization:** Gradient
Date: 6/2/2022	**Date:** 6/2/2022
	Name: Kim Reid
	Title: Principal Scientist
	Organization: Gradient
	Date: 6/2/2022
	Name: Tom Lewandowski, Ph.D., DABT, ERT, ATS
	Title: Principal
	Organization: Gradient
	Date: 6/2/2022
Assessor Type (Licensed GreenScreen Profiler, Authorized GreenScreen Practitioner, or Unaccredited):	Licensed GreenScreen Profiler

Confirm Application of the Disclosure and Assessment Rules and Best Practice:[3] N/A

Chemical Name (CAS #): 1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy) (CAS # 25713-60-4)

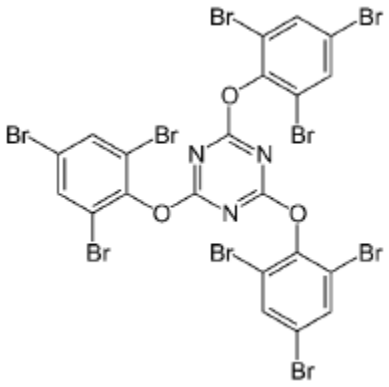
Molecular Formula: $C_{18}H_4Br_8N_2O_4$

[1] Use GreenScreen Assessment Procedure (Guidance) v1.4 (January 2018).
[2] GreenScreen reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen Practitioner), "CERTIFIED" (by Licensed GreenScreen Profiler or equivalent), or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen Verification Program).
[3] See GreenScreen Guidance v1.4.

SMILES: c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br

Also Called: Tris(tribromophenoxy)triazine (TTBPT)

Chemical Structure:



Source: NLM (2021).

Suitable Analogs or Moieties Used in This Assessment (CAS #s): N/A

Notes Related to Production-Specific Attributes:[4] N/A

For Inorganic Chemicals and Relevant Particulate Organics: N/A

Define Properties:

1. **Particle Size:** <10 µm (4%) and 10-100 µm (63%) (NICNAS, 2006). D50 = <100 µm (ICL-IP Europe B.V., 2017). D50 = 97.9 µm (ECHA, 2021). High molecular weight (MW) = 1,067.43.
2. **Structure:** Solid, powder (NICNAS, 2006; ECHA, 2021).
3. **Mobility (*e.g.*, Water Solubility, Volatility):**
   a. Water Solubility: <1E-3 mg/L at 20°C (NICNAS, 2006; ECHA, 2021).
   b. Vapor Pressure: 1.52E-23 kPa at 25°C (NICNAS, 2006; ICL-IP Europe B.V., 2017).
   c. Adsorption/Desorption: Log K_{oc} = 9.53 at 35°C (ECHA, 2021). Log K_{oc} = 7.6 (estimated) (NICNAS, 2006).
4. **Bioavailability:**
   a. K_{ow}: Log P_{ow} = 8.63 (ECHA, 2021; ICL-IP Europe B.V., 2017). Log P_{ow} = >5.85 (NICNAS, 2006). Log K_{ow} = >10 (estimated using KOCWIN version 2.0; US EPA, 2021a).

[4] 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, byproducts or transformation products. Explain any differences between the manufactured chemical product and the GreenScreen assessment of the generic chemical by CAS #.

Identify Applications/Functional Uses (*e.g.*, Cleaning Product, TV Casing):

1. Flame retardant in electronics (NICNAS, 2006).
2. Polymer applications in acrylonitrile-butadiene-styrene (ABS) and high-impact polystyrene (HIPS) (NICNAS, 2006).

GreenScreen Benchmark Score and Hazard Summary Table[5]

1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy) (hereafter, TTBPT) is assigned a Benchmark Score of BM-2 based on *Very High (vH)* persistence and *Moderate (M)* endocrine activity. The *Moderate (M)* score for endocrine activity is based on TTBPT's presence on the OSPAR Commission Priority PBTs and EDs and Equivalent Concern[9] screening list. However, the confidence in this score is low due to a lack of data to confirm the evidence of endocrine activity for TTBPT. The data requirements were met for the BM-2 classification, as shown in Table 1, below.

Table 1 GreenScreen (v1.4) Hazard Profile Summary Table – 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy) (CAS # 25713-60-4)

Group I Human					Group II and II* Human									Ecotox.		Fate		Phys.	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						slg	rpt*	slg	rpt*										
L	*L*	*L*	**L**	*M*	**L**	**L**	**L**	*L*	**L**	**L**	*L*	**L**	**L**	**L**	*L*	*vH*	*L*	**L**	**L**

Notes:
CAS = Chemical Abstracts Service.
Hazard levels (Very High [vH], High [H], Moderate [M], Low [L], Very Low [vL]) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence.
Hazard levels in **bold** font reflect 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.
Hazard endpoint acronym definitions are provided in Appendix A.

Environmental Transformation Products and Ratings[10]

Identify feasible and relevant environmental transformation products (*i.e.*, dissociation products, transformation products, valence states) and/or moieties of concern (Table 2).[11]

[5] See Appendix A for a glossary of hazard endpoint acronyms.
[6] See Appendix B for alternative GreenScreen Hazard Summary Table (in which classifications are presented by exposure route).
[7] For inorganic chemicals only, see GreenScreen Guidance v1.4 Section 12. (Exceptions for Persistence).
[8] For systemic toxicity and neurotoxicity, repeated-exposure data are preferred. A lack of single-exposure data is not a data gap when repeated-exposure data are available. In that case, a lack of single-exposure data may be represented as NA instead of DG. See GreenScreen Guidance v1.4 Section V, Annex 2, 2.3 (A2.2.3).
[9] PBT = Persistent, Bioaccumulative, and Toxic. ED = Endocrine Disruptor.
[10] See GreenScreen Guidance v1.4 Sections 11.4 and 11.5.
[11] 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.

Table 2 Environmental Transformation Products and Ratings

Functional Use	Life Cycle Stage	Transformation Pathway	Environmental Transformation Products	CAS #	Feasible and Relevant?	GreenScreen List Translator Score or GreenScreen Benchmark Score
N/A	Degradation	Cleavage of the ether linkages	Tribromophenol (TBP)	118-79-6	Minimal breakdown product (thus of unclear relevance)	LT-1 (Likely Benchmark 1)

Notes:
CAS = Chemical Abstracts Service; N/A = Not Applicable.
Source: ECHA (2021).

Introduction

TTBPT is a brominated flame retardant commonly used in plastics and electronics. Common applications for TTBPT-containing plastics include computer monitors, televisions, videos, remote controls, mobile phones, and office equipment. TTBPT is not sold directly to the general public and is handled in its pure form mostly in manufacturing/industrial settings (NICNAS, 2006). Table 3 summarizes the physical and chemical properties obtained for TTBPT.

Table 3 Physical and Chemical Properties of 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy)

Property	Value	Reference
Molecular Formula	$C_{12}H_6Br_9N_3O_3$	Expert judgment
SMILES Notation	C1=C(C=C(C(=C1Br)OC2=NC(=NC(=N2)OC3=C(C=C(C=C3Br)Br)Br)OC4=C(C=C(C=C4Br)Br)Br)Br)Br	NLM (2021)
Molecular Weight	1,067.4 g/mol	NLM (2021)
Physical State	Solid at 20°C and 1,013 hPa	ECHA (2021)
Appearance	White solid powder	NICNAS (2006); ECHA (2021)
Melting Point	228-229°C	ECHA (2021)
Vapor Pressure	0 Pa (25°C)	ECHA (2021)
	1.52E-23 kPa at 25°C	NICNAS (2006); ICL-IP Europe B.V. (2017)
Water Solubility	0.001 mg/L (20°C)	NICNAS (2006); ECHA (2021)
Dissociation Constant	Not applicable	Expert judgment
Density/Specific Gravity	2.44 g/mL (20°C)	ECHA (2021)
Partition Coefficient (Log K_{ow})	>5.8 (20°C)	NICNAS (2006); ECHA (2021)

Notes:
SMILES = Simplified Molecular-Input Line-Entry System.
Gradient assessed Chemical Name against GreenScreen version 1.4 (Clean Production Action, 2019).

Hazard Classification Summary Section

Hazard classifications for the GreenScreen endpoints evaluated are provided below.

Group I Human Health Effects (Group I Human)

Carcinogenicity (C)

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

TTBPT is assigned a score of *Low* (*L*) for carcinogenicity, with low confidence. This score is based on negative genotoxicity data, an assessment of *in silico* predictions for carcinogenicity, and professional judgment. The chemical did not trigger any structural alerts for genotoxic or nongenotoxic carcinogenicity using Toxtree, but was determined to be of low to moderate concern for carcinogenicity based on OncoLogic. TTBPT is not present on any authoritative or screening lists. Furthermore, the chemical did not induce histopathological effects in a subchronic oral study in rats and has been shown to have limited bioavailability in rats. This classification is made with low confidence because it is not based on experimental carcinogenicity data.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- TTBPT was not mutagenic in three *in vitro* studies: an Organisation for Economic Co-operation and Development (OECD) Test Guideline (TG) 471 bacterial reverse mutation assay, an OECD TG 473 mammalian chromosome aberration test, and an OECD TG 476 mammalian cell gene mutation test (ECHA, 2021).
- TTBPT did not induce histopathological changes in rats exposed to up to 1,000 mg/kg-bw/day *via* oral gavage for 13 weeks. No neoplastic or pre-neoplastic changes indicative of a carcinogenic effect were noted in this OECD guideline study (Charles River, 2009).
- Based on the chemical structure of TTBPT, it is considered a halogenated aromatic. Although a number of halogenated aromatics have been shown to be carcinogenic in experimental animals, the mechanism of their carcinogenic action is not clearly understood. The final level of carcinogenicity concern for this compound was determined to be low-moderate (US EPA, 2021b).
- TTBPT is predicted by the expert rule-based *in silico* program Toxtree version 3.1.0 (Ideaconsult Ltd., 2018) to be noncarcinogenic *via* a nongenotoxic, nonmutagenic mechanism (US EPA, 2021c).

Mutagenicity/Genotoxicity (M)

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

TTBPT is assigned a score of *Low (L)* for mutagenicity, with low confidence. The three *in vitro* studies reviewed indicate that TTBPT is not mutagenic or clastogenic. In addition, TTBPT is not present on any authoritative or screening lists. This classification is made with low confidence based on a lack of *in vivo* experimental studies.

Authoritative and Screening Lists

- **Authoritative**: Not listed.
- **Screening**: Not listed.

Studies

- **NICNAS (2006):**
  - TTBPT was not mutagenic in an *in vitro* bacterial reverse mutation assay (1997; OECD TG 471), both with and without metabolic activation (S9 mix), conducted using *Salmonella typhimurium* strains TA1535, TA1537, TA98, and TA100. TTBPT doses in this study ranged from 10 to 1,000 μg/plate. An appropriate solvent (dimethyl sulfoxide [DMSO]) and positive controls were evaluated concurrently in both the absence and presence of metabolic activation. Under the test conditions, TTBPT was negative for mutagenicity both with and without metabolic activation. No cytotoxicity was observed up to the maximum dose. Control groups responded appropriately, validating the study results.
  - TTBPT was not mutagenic in an *in vitro* mammalian cell gene mutation test (1997; OECD TG 476), both with and without metabolic activation (S9 mix), conducted using mouse lymphoma cells (L5178Y). TTBPT doses in this study ranged from 0.025 to 100 μg/mL (in DMSO). Both positive and negative control values were reported to be within acceptable limits. Under the test conditions, TTBPT was negative for mutagenicity both with and without metabolic activation. Precipitation of the test substance was reported at the maximum dose of 100 μg/mL, but no cytotoxicity was observed up to the maximum dose. Control groups responded appropriately, validating the study results.
  - TTBPT was not clastogenic in an *in vitro* chromosome aberration assay (1997; OECD TG 473), both with and without metabolic activation (S9 mix), conducted using cultured peripheral human lymphocytes. TTBPT doses in this study ranged from 0.1 to 10 μg/mL (in DMSO). Positive controls were evaluated concurrently. No cytotoxicity was observed at the highest dose tested (10 μg/mL). TTBPT did not increase the number of cells with chromosome aberrations both with and without metabolic activation. Control groups responded appropriately, validating the study results.

Reproductive Toxicity (R)

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

TTBPT is assigned a score of *Low (L)* for reproductive toxicity, with low confidence. This score is based on a lack of treatment-related changes in sperm count, sperm motility, estrus cycle, or effects on reproductive organs and tissues in rats treated with up to 1,000 mg/kg-bw/day of TTBPT in comparison to control animals in an OECD guideline 90-day subchronic toxicity study in which the test substance was administered *via* the oral route. Confidence in this score is low because although the experimental data available for the test substance is reliable, the cited study is a repeated-dose toxicity study that also evaluated various reproductive parameters. There is no reproductive toxicity-specific study available or human data to support the weight of the evidence. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **ICL-IP Europe B.V. (2017) and Charles River (2009):**
  - In a subchronic repeated-dose toxicity test (2009; OECD TG 408), Sprague-Dawley rats (n = 10/sex/dose) were administered 0, 100, 350, or 1,000 mg/kg-day of TTBPT *via* oral gavage for 13 weeks, followed by a 28-day recovery period. No significant adverse effects, including effects on clinical signs, mortality, body weight, food and water consumption, ophthalmology, hematology, clinical biochemistry, organ weights, gross pathology, or histopathology, were noted. There were no effects on sperm count, sperm motility, or estrus cycle parameters. In addition, no adverse effects on reproductive organs or tissues were observed. A no observed adverse effect level (NOAEL) of greater than 1,000 mg/kg-bw/day was determined.

Developmental Toxicity, Including Developmental Neurotoxicity (D)

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

TTBPT is assigned a score of **Low (L)** for developmental toxicity, with high confidence. This score is based on the lack of observed developmental effects from an OECD guideline prenatal developmental toxicity study in rats. This score is assigned with high confidence because it is based on reliable experimental data for TTBPT. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **ECHA (2021) and KTR (2013):**
  - In a pre-natal developmental toxicity study (OECD TG 414), pregnant Sprague-Dawley rats (n = 21 females/dose) were administered 250, 500, or 1,000 mg/kg-day of TTBPT (in carboxymethylcellulose) *via* oral gavage from gestational day 5 to 19. No changes in maternal body weight or food consumption were observed. No treatment-related changes in gravid uterine weight, numbers of corpora lutea or implantation, implantation index, or pre- or post-implantation losses were observed in any of the treatment groups. In addition, no significant treatment-related effects on embryo-fetal survival, growth, or development were noted. Based on the results of this study, a NOAEL for developmental toxicity 1,000 mg/kg-bw/day was determined.

Endocrine Activity (E)

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

TTBPT is assigned a score of *Moderate (M)* for endocrine activity, with low confidence. This classification is based on the presence of TTBPT on a screening list for endocrine activity (OSPAR Commission Priority PBTs and EDs and Equivalent Concern). Confidence in this score is low because there is a lack of experimental data in animals for TTBPT.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** OSPAR – Priority PBTs & EDs & Equivalent Concern – Endocrine Disruptor – Chemical for Priority Action.

Studies

- **US EPA (2021d):**
  - TTBPT has not been screened through the United States Environmental Protection Agency (US) EPA Endocrine Disruptor Screening Program (EDSP) for Estrogen Receptor Bioactivity as of December 3, 2021 (US EPA, 2021d).

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

Note: *Group II and Group II* endpoints are distinguished in the v1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. When classifying hazard for Systemic Toxicity/Organ Effects and Neurotoxicity endpoints, repeated exposure results are required and preferred. Lacking repeated exposure results in a data gap. Lacking single exposure data does not result in a data gap when repeated exposure data are present (shade out the cell in the hazard table and make a note). If data are available for both single and repeated exposures, then the more conservative value is used.*

Acute Mammalian Toxicity (AT) Group II

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

TTBPT is assigned a score of **Low (L)** for acute mammalian toxicity, single exposure, with high confidence. This score is based on the results of two OECD guideline acute toxicity studies in which median lethal doses (LD_{50} values) were reported at values greater than would warrant classification per Globally Harmonized System of Classification and Labeling of Chemicals (GHS) guidelines. No mortalities were observed in these studies. The oral and dermal LD_{50} values were both >2,000 mg/kg bw and the inhalation median lethal concentration (LC_{50}) was >1.47 mg/L (dust). Confidence in this score is high because it is based on reliable experimental data for TTBPT for all three routes of exposure. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Oral

- **NICNAS (2006):**
  - In an acute oral toxicity study (1997; OECD TG 401), male and female Sprague-Dawley rats (n = 5/sex) were administered a single dose of 2,000 mg/kg bw TTBPT (in 1% aqueous carboxymethyl cellulose) *via* oral gavage and observed for at least 2 days. Hunched posture and was noted in all of the females and one male, and piloerection was noted in two females and one male, but these effects were reversed by day 2 of observation. No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the oral route of exposure.

Dermal

- **NICNAS (2006):**
  - In an acute dermal toxicity study (1997; OECD TG 402), male and female Wistar rats (n = 5/sex) were administered 2,000 mg/kg bw of TTBPT (in 1% aqueous carboxymethyl cellulose) dermally (occluded). No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the dermal route of exposure.

Inhalation

- **ECHA (2021) and ICL-IP Europe B.V. (2017):**
  - In an acute inhalation toxicity study (2011; OECD TG 403; Klimisch score [K] = 1), male and female Sprague-Dawley rats (n = 5/sex) were administered 1.47 mg/L of TTBPT *via* the nose

only for 4 hours. No details on clinical signs observed or mortality were reported. The LC_{50} was determined to be greater than 1.47 mg/L. Due to a lack of study details, the acute toxicity of the test substance *via* the inhalation route of exposure cannot be reliably determined. However, the reported LC_{50} value of >1.47 mg/L suggests low or moderate toxicity.

- **NICNAS (2006):**
  - According to the Australia National Industrial Chemicals Notification and Assessment Scheme (NICNAS), "TTBPT is not considered respirable, with only 4% of particles having less than 10 μm diameter" (NICNAS, 2006).

Systemic Toxicity/Organ Effects, Including Immunotoxicity (ST)

(ST-Single) Group II

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

TTBPT is assigned a score of **Low (L)** for single-exposure systemic toxicity/organ effects, including immunotoxicity, with high confidence. This score is based on an acute oral, dermal, and inhalation toxicity studies in rats. No clinical signs or adverse pathological effects indicative of specific-target-organ toxicity were reported in these studies. Confidence in this score is high, because it is based on reliable experimental data for TTBPT for all three routes of exposure. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Oral

- **NICNAS (2006):**
  - In an acute oral toxicity study (1997; OECD TG 401), male and female Sprague-Dawley rats (n = 5/sex) were administered a single dose of 2,000 mg/kg bw of TTBPT (in 1% aqueous carboxymethyl cellulose) *via* oral gavage and observed for at least 2 days. Hunched posture and was noted in all of the females and one male, and piloerection was noted in two females and one male, but these effects were reversed by day 2 of observation. No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the oral route of exposure.

Dermal

- **NICNAS (2006):**
  - In an acute dermal toxicity study (1997; OECD TG 402), male and female Wistar rats (n = 5/sex) were administered 2,000 mg/kg bw of TTBPT (in 1% aqueous carboxymethyl cellulose) dermally (occluded). No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the dermal route of exposure.

Inhalation

- **ECHA (2021) and ICL-IP Europe B.V. (2017):**
  - In an acute inhalation toxicity study (2011; OECD TG 403; K = 1), male and female Sprague-Dawley rats (n = 5/sex) were administered 1.47 mg/L of TTBPT *via* the nose only for 4 hours. The LC_{50} was determined to be greater than 1.47 mg/L, but no details on clinical signs observed, mortality, or necropsy results were reported (Weniger, 2011, as cited in ICL-IP Europe B.V., 2017).

(ST-Repeated) Group II*

Score (H, M, or L): L

TTBPT is assigned a score of **Low (L)** for repeated-exposure systemic toxicity/organ effects, including immunotoxicity, with high confidence. This score is based on 28-day and 90-day subchronic repeated-dose studies in rats administered TTBPT *via* oral gavage. No adverse treatment-related effects were noted in these studies at doses up to 1,000 mg/kg-bw/day. Confidence in this score is high because it based on reliable experimental data for TTBPT. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Oral

- **Charles River (2009) and ICL-IP Europe B.V. (2017):**
  - In a subchronic repeated-dose toxicity test (2009; OECD TG 408), Sprague-Dawley rats (n = 10/sex/dose) were administered 0, 100, 350, or 1,000 mg/kg-day of TTBPT *via* oral gavage for 13 weeks, followed by a 28-day recovery period. No significant adverse effects, including effects on clinical signs, mortality, body weight, food and water consumption, ophthalmology, hematology, clinical biochemistry, organ weights, gross pathology, or histopathology, were noted. In addition, no adverse effects on reproductive organs or tissues were observed. A

NOAEL of greater than 1,000 mg/kg-day was established (Charles River, 2009; ICL-IP Europe B.V., 2017).

- In a non-standard 28-day oral gavage toxicity study, rats (n = 6/sex/group) were administered TTBPT at doses of 0, 10, 50, 250, or 1,000 mg/kg-bw/day for 28 days, with a 14-day follow-up period. No mortality was observed. Some incidental findings (hair loss, tail wounds, and scab formation) were noted during daily observations, but these effects were not considered treatment related. Body weight gain was not affected by the treatment. In terms of serum chemistry, a significant decrease (33%, $p < 0.05$) in the liver enzyme gamma glutamyl transpeptidase (GGT) was seen in high-dose recovery males when compared to controls, but not in males at the end of treatment. A significant decrease (10%, $p < 0.05$) in serum albumin/globulin ratio was observed in high-dose recovery females when compared to controls. Minor changes in hematology (*e.g.*, mean corpuscular hemoglobin levels and an increase in mean corpuscular volume) were noted, but did not show a clear dose-response pattern. Some statistically significant differences in relative adrenal, liver, and kidney weights were also observed, but these effects likewise did not follow a dose-response pattern. Overall, observed differences in hematology, blood chemistry, organ weights, clinical signs, gross pathological findings, and histopathological findings were considered unrelated to TTBPT treatment, due to the lack of clear dose-response patterns, occurrence in only one or two animals in a treatment group, and the occurrence of similar changes in controls. The NOAEL in this study was reported as 1,000 mg/kg-bw/day (Yamasaki, 1990, as cited in ICL-IP Europe B.V., 2017).

Inhalation

- None.

Dermal

- None.

Neurotoxicity (N)

Neurotoxicity (N) Group II – Single

Score (vH, H, M, or L): *L*

TTBPT is assigned a score of *Low (L)* for neurotoxicity *via* a single exposure, with low confidence. This score is based on a lack of neurotoxic effects observed in OECD guideline acute toxicity tests *via* the oral and dermal routes. Confidence in this score is low because although the experimental data for the test substance were reliable, no specific assessments of neurotoxicity were conducted in the identified studies and there is a lack of human data to support the weight of the evidence. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Oral

- **NICNAS (2006):**
  - In an acute oral toxicity study (1997; OECD TG 401), male and female Sprague-Dawley rats (n = 5/sex) were administered a single dose of 2,000 mg/kg bw of TTBPT (in 1% aqueous carboxymethyl cellulose) via oral gavage and observed for at least 2 days. Hunched posture and was noted in all of the females and one male, and piloerection was noted in two females and one male, but these effects were reversed by day 2 of observation. No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the oral route of exposure.

Dermal

- **NICNAS (2006):**
  - In an acute dermal toxicity study (1997; OECD TG 402), male and female Wistar rats (n = 5/sex) were administered 2,000 mg/kg bw of TTBPT (in 1% aqueous carboxymethyl cellulose) dermally (occluded). No signs of systemic toxicity were observed and no mortality occurred. The LD_{50} was determined to be greater than 2,000 mg/kg bw. This study indicated that the test substance exhibits low acute toxicity *via* the dermal route of exposure.

Inhalation

- **ECHA (2021):**
  - In an acute inhalation toxicity study (2011; OECD TG 403; K = unspecified), male and female Sprague-Dawley rats (n = unspecified/sex) were administered an unknown concentration of TTBPT *via* the nose only for 4 hours. The LC_{50} was determined to be greater than 1.47 mg/L, but no details on clinical signs observed, mortality, or necropsy results were reported.

Neurotoxicity (N) Group II* – Repeated

Score (H, M, or L): L

TTBPT is assigned a score of **Low (L)** for neurotoxicity *via* repeated exposure with high confidence. This score is based on results from a 91-day subchronic toxicity study in which no neurotoxic effects were observed in rats administered doses up to 1,000 mg/kg-day. No neurological effects were observed in this study, in which neurological endpoints were assessed (*e.g.*, *via* a functional observation battery) following repeated exposures. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Oral

- **Charles River (2009) and ICL-IP Europe B.V. (2017):**
  - In a subchronic repeated-dose toxicity test (2009; OECD TG 408), Sprague-Dawley rats (n = 10/sex/dose) were administered 0, 100, 350, or 1,000 mg/kg-day of TTBPT *via* oral gavage for 13 weeks, followed by a 28-day recovery period. In addition to systemic endpoints, neurotoxicity was also investigated following the standard study protocol. Cage-side observations, including prostration, lethargy, tremors, and convulsions, were examined once during the pretrial period (Week 1) and weekly thereafter for all of the test animals. In addition, functional tests, including grip strength, pain perception, landing foot splay, and motor activity, were performed once during the pretrial period (Week 1), during Weeks 4 and 12 of treatment, and during Week 4 of the recovery period. Repeated exposures to TTBPT did not cause any functional abnormality. The NOAEL for repeated-dose systemic toxicity was 1,000 mg/kg-day in this study (Charles River, 2009; ICL-IP Europe B.V., 2017).

Skin Sensitization (SnS) Group II*

Score (H, M, or L): L

TTBPT is assigned a **Low (L)** score for skin sensitization, with high confidence. This score is based on a lack of skin sensitization reactions in a guinea pig maximization test, supported by a lack of structural alerts for skin sensitization predicted using the expert rule-based *in silico* programs Toxtree and Derek Nexus. Confidence in this score is high because it is based on reliable experimental data and supported by *in silico* predictions. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **NICNAS (2006):**
  - In a guinea pig maximization test (1997; OECD TG 406), researchers applied TTBPT to female Himalayan guinea pigs at 5% in corn oil for intradermal induction, 50% in corn oil for the topical induction, and 50% in corn oil for the topical challenge exposures. Animals were divided among two groups: test animals (n = 20) and controls (n = 10). Mortality (n = 2) was observed on days 6 and 7 of the study. Macroscopic post-mortem examination showed that both of these animals showed dark red discoloration of the lungs. Mild to moderate erythema was observed at 24 hours in one of the animals in the test group. It was noted that the same guinea pig exhibited a reaction to the vehicle (corn oil), while none of the guinea pigs in the control group exhibited any reactions. After 48 hours, there were no reactions in either group. A sensitization rate of 0-6% was reported in this study. The test substance was deemed non-sensitizing under the test conditions, based on a response rate <30%.

Modeled Data

- The predictive toxicology program Derek Nexus version 6.1.0 predicted TTBPT to be a non-sensitizer, with no misclassified or unclassified features (Lhasa Ltd., 2016).
- Toxtree version 3.1.0 identified no structural alerts for skin sensitization associated with the chemical structure of TTBPT (Ideaconsult Ltd., 2018).

Respiratory Sensitization (SnR) Group II*

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

TTBPT is assigned a *Low (L)* score for respiratory sensitization, with low confidence. This score is based on a lack of OECD Quantitative Structure-Activity Relationship (QSAR) Toolbox structural alerts for respiratory sensitization and a lack of experimental data on respiratory sensitization in humans or animals from TTBPT exposure. Additionally, TTBPT is not considered respirable based on the fact that 4% of its particles are less than 10 μm in diameter (NOTOX, 1997, as cited in NICNAS, 2006). Furthermore, TTBPT is not present on any authoritative or screening lists. Confidence in this score is low because the classification is based on a weight-of-evidence approach and because TTBPT lacks experimental data for this endpoint.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Modeled Data

- No mechanism-based structural alerts were predicted by the predictive toxicology program OECD QSAR Toolbox version 4.4.1 (OECD, 2021; see Appendix D).

Skin Irritation/Corrosivity (IrS) Group II

Score (vH, H, M, or L): **L**

TTBPT is assigned a score of **Low (L)** for skin irritation/corrosivity, with high confidence. This score is based on the results of a skin irritation study conducted in rabbits. Confidence in this score is high because it is based on reliable experimental data for TTBPT. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **NICNAS (2006) and ECHA (2021):**
  - In a skin irritation study (1997; OECD TG 404), TTBPT (moistened with distilled water) was applied to the skin of New Zealand white rabbits (n = 3) under semi-occlusive conditions, and the animals were observed for a period of 72 hours. No dermal reactions (erythema or edema) were noted in any animals throughout the duration of the study, and the test substance was determined to be non-irritating to the skin.

Eye Irritation/Corrosivity (IrE) Group II

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

TTBPT is assigned a score of **Low (L)** for eye irritation/corrosivity, with high confidence. This score is based on a lack of effects observed in an eye irritation study conducted in rabbits. Confidence in this score is high because it is based on reliable experimental data for TTBPT. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **NICNAS (2006):**
  - In an eye irritation study (1997; OECD TG 405), TTBPT (undiluted) was instilled into the right eye of New Zealand white rabbits (n = 3). Observations were conducted at 24, 48, and 72 hours following test item application. Conjunctival redness (score = 2) was observed in the test animals at 24 hours, but this resolved for all of the animals by 48 hours. Conjunctival chemosis (score = 1) was observed in the test animals at 24 hours, but this also resolved for all of the animals by 48 hours. No inflammation of the iris or corneal effects were observed at any time point. Thus, TTBPT was determined to be non-irritating to the eyes of rabbits under the conditions of this study.

Ecotoxicity (Ecotox.)

Acute Aquatic Toxicity (AA)

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

TTBPT is assigned a score of **Low (L)** for acute aquatic toxicity, with high confidence. This assignment is based on experimental algae, invertebrate, and fish toxicity data for TTBPT (Table 4). No adverse effects were observed at concentrations up to the water solubility of TTBPT (*i.e.*, 0.001 mg/L at 20°C). Therefore, TTBPT exhibits low acute aquatic toxicity in accordance with GreenScreen guidance. The score is assigned

with high confidence because the studies relied upon were conducted following OECD guidelines. In addition, TTBPT is not present on any authoritative or screening lists.

Authoritative and Screening Lists

- **Authoritative**: Not listed.
- **Screening:** Not listed.

Studies

Table 4 Acute Aquatic Toxicity Data for 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy)

Trophic Level	Test Species	Method	Test Type (K)	Endpoint (Basis)	Value (mg/L)	Source
Algae	Algae (*Selenastrum capricornutum*)	OECD TG 201	Static freshwater (Unspecified)	72-hour ErC_{50} (growth rate and biomass)	>1	NICNAS (2006)
Invertebrate	Water Flea (*Daphnia magna*)	OECD TG 202	Static freshwater (Unspecified)	48-hour LC_{50} (mobility)	>0.37	
Fish	Carp (*Cyprinus carpio*)	OECD TG 203	Static freshwater (Unspecified)	96-hour LC_{50}	>0.37	
Algae	Algae (*Pseudokirchneriella subcapitata*)	Unspecified	Static freshwater (Unspecified)	72-hour ErC_{50} (growth rate and biomass)	>0.013	ECHA (2021)
Invertebrate	Water Flea (*Daphnia magna*)	Unspecified	Static freshwater (Unspecified)	48-hour EC_{50} (mobility)	>0.013	
Fish	Unspecified	Unspecified	Semistatic freshwater (Unspecified)	96-hour LC_{50} (mortality)	>0.013	

Notes:
EC_{50} = Median Effect Concentration; ErC_{50} = Concentration that Results in a 50% Reduction in Growth Rate Relative to Controls; K = Klimisch Score; LC_{50} = Median Lethal Concentration; OECD TG = Organisation for Economic Co-operation and Development Test Guideline.

Chronic Aquatic Toxicity (CA)

Score (vH, H, M, or L): *L*

TTBPT is assigned a score of *Low (L)* for chronic aquatic toxicity, with low confidence, based on a study of one trophic-level (algae) with experimental toxicity data on this endpoint (Table 5), a mammalian oral absorption, distribution, metabolism, and excretion (ADME) study, and an 8-week bioaccumulation study in red killifish (*Oryzias latipes*). Confidence in this score is low because experimental data from only one trophic-level study was identified. Though both the algae study and the 8-week bioaccumulation study data for TTBPT are reliable, these studies were performed above the practical saturation limit for TTBPT. Overall, based on TTBPT's low water solubility and expected limited bioavailability, the potential for chronic aquatic toxicity is low. In addition, TTBPT is not present on any authoritative or screening lists for chronic aquatic toxicity.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

Table 5 Chronic Aquatic Toxicity Data for 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy)

Trophic Level	Test Species	Method	Test Type (K)	Endpoint (Basis)	Value (mg/L)	Source
Algae	Algae (*Pseudokirchneriella subcapitata*)	Unspecified	Static freshwater (Unspecified)	72-hour NOEC (growth rate and biomass)	>0.013	ECHA (2021)

Notes:
K = Klimisch Score; NOEC = No Observed Effect Concentration.

- **NICNAS (2006) and ICL-IP Europe B.V. (2017):**
  - In a bioaccumulation study performed using test methods for new chemical substances (Kanpogyo No. 5 Yakuhatsu No. 615, 49 Kikyoku No. 392, 1974), red killifish (*Oryzias latipes*) were exposed to nominal concentrations of TTBPT (CAS # 25713-60-4) at 0.5 or 0.05 mg/L for 8 weeks using a continuous flow-through system. Analytical monitoring was performed using high-performance liquid chromatography (HPLC). The bioconcentration factors (BCFs) were determined to be <0.8-9 and 8.0-18 for 0.5 and 0.05 mg/L, respectively (Kurume Research Laboratory, 1990b, as cited in NICNAS, 2006). The study authors concluded that TTBPT is "not bioaccumulative in the food chain as the BCF criteria are not exceeded. Further, the notified chemical high molecular weight and low water solubility suggests that it is unlikely to cross biological membranes and bioaccumulate (Connell 1990). Release to the aquatic environment will be very limited from the proposed uses and thus aquatic toxicity is unlikely to occur" (NICNAS, 2006). However, according to ICL-IP Europe B.V (2017), the "[f]ish were exposed to 0.5 mg/l which is much above the maximum level of water solubility of the substance. Therefore, although no bioconcentration was observed, valid results cannot be derived due to the concentrations used."
- **ICL-IP Europe B.V. (2017) and Huntingdon Life Sciences Ltd. (2006):**
  - In a mammalian oral ADME study (OECD TG 417), Sprague-Dawley rats (n = 12/sex/dose) were administered a single dose of 50 or 1,000 mg/kg-day of radiolabeled TTBPT suspended in 0.5% carboxymethycellulose *via* gastric intubation. The radiolabeled TTBPT was entirely excreted *via* the feces (95.4-105%), with the majority excreted within the interval of 0-48 hours. Very low amounts of radioactivity were found in the urine (0.2%), expired air (<0.1%), carcass (<0.01% of the low dose; 0.03-1.27% of the high dose), and cage washes (0.01-0.26%). The total absorption was estimated to be 0.2% of the administered dose. Based on the study findings, it was concluded that TTBPT is not likely to be absorbed or accumulate in biological tissues.

Environmental Fate (Fate)

Persistence (P)

Score (vH, H, M, L, or vL): vH

TTBPT is assigned a score of **Very High (vH)** for persistence, with high confidence. TTBPT is insoluble in water (*i.e.*, water solubility is <0.001 mg/L); thus, it is not available for biotic or abiotic degradation. A biodegradation study in water found that TTBPT is neither readily nor inherently biodegradable. Due to its very low vapor pressure ($<1 \times 10^{-5}$ Pa) and insolubility in water, air and water are not considered environmental compartments of concern for TTBPT. Given its propensity to bind to solids (experimental log K_{oc} = 9.53; modeled log K_{oc} = 7.25), TTBPT is expected to primarily amass in soil and sediment (ECHA, 2021). The modeled half-life of TTBPT in soil is 360 days, indicating high persistence. The modeled half-life of TTBPT in sediment is 1,621 days, indicating very high persistence. The soil half-life is used as the basis for the persistence hazard score, because TTBPT is predicted to primarily distribute to soil. Confidence in this score is high because it is based on both experimental studies and modeled data.

Authoritative and Screening Lists

- **Authoritative:** None.
- **Screening:** None.

Studies

- **ECHA (2021) and NICNAS (2006):**
  - A ready biodegradability study (1997) was conducted with TTBPT under aerobic aqueous conditions, using a domestic, nonadapted activated sludge mixture of sewage, soil, and natural water. After 28 days, an initial concentration of 100 mg/L resulted in greater than 4 but less than 6% degradation. The test substance was determined to be not readily biodegradable (Kurume Research Laboratories, 1990a, as cited in NICNAS, 2006; ECHA, 2021).
  - An inherent biodegradability study (2005; OECD TG 302 D) was conducted with TTBPT under aerobic aqueous conditions, using a buffer mineral salts medium. After 74 days, an initial concentration of 20 mg/L resulted in 4% degradation measured by carbon dioxide (CO_2) evolution in sealed bottles. The test substance was determined to be not inherently biodegradable (IMI-TAMI, 2004, as cited in NICNAS, 2006; ECHA, 2021).
- **ECHA (2021):**
  - A sediment simulation study (2009; OECD TG 308) was conducted with TTBPT under aerobic aqueous conditions, using natural water and sediment. After 100 days, an initial concentration of 0.07 mg/L resulted in 17.3% degradation by radiochemical analysis. The disappearance times (DT_{50}) in the sediment layers were 472 and 592 days, respectively.
  - A sediment simulation study (2009; OECD TG 308) was conducted with TTBPT under anaerobic aqueous conditions, using natural water and sediment. After 100 days, an initial concentration of 0.071 mg/L resulted in 19.8% degradation by radiochemical analysis. The DT_{50} in the sediment layers were 252 and 462 days, respectively.

Modeled Data

Environmental partitioning behavior and half-lives for TTBPT were modeled using the Epi Suite Level III fugacity model. These values are presented in Table 6. TTBPT is expected to primarily amass in soil (92.9%) and water (4.17%). See Appendix C for modeling results.

Table 6 Modeled Environmental Partitioning and Half-Life for 1,3,5-Triazine, 2,4,6-Tris(2,4,6-tribromophenoxy) Using EPI Suite Version 4.11

Compartment	Mass Amount (%)	Half-Life (Hours)	Half-Life (Days)	Model	Source
Air	0.105	173	7.2	Level III fugacity model	US EPA (2021a)
Water	4.17	4,320	180		
Soil	92.9	8,640	360		
Sediment	2.79	38,900	1,620.8		

Notes:
Log P_{ow} = Ratio of Equilibrium Concentrations of a Dissolved Substance in n-Octanol and Water; SMILES = Simplified Molecular-Input Line-Entry System.
Values were modeled in EPI Suite version 4.11 using the SMILES notation and modeled values for water solubility (1.849E-011 mg/L), log P_{ow} (11.46), and melting point (338°C).

Bioaccumulation (B)

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

TTBPT is assigned a score of *Low (L)* for bioaccumulation, with low confidence, based on its molecular weight and low water solubility, as well as the results of a mammalian oral ADME study in rats, all of which indicate that TTBPT has a low bioaccumulation potential. This score is assigned with low confidence because although the reviewed fish BCF study for TTBPT indicates that it has a low bioaccumulation potential, the test concentrations were above the practical saturated limit for TTBPT. Moreover, the results of the ADME study indicate an absence of significant uptake of TTBPT (ICL-IP Europe B.V., 2017; Huntingdon Life Sciences Ltd., 2006), suggesting minimal bioaccumulation. It is noteworthy that its experimental K_{oc} (9.53) indicates that the potential for TTBPT to migrate into water is negligible, and thus, TTBPT is not likely to be bioavailable to aquatic species. Furthermore, an activated sludge respiration inhibition test and two sediment toxicity studies (OECD TGs 225 and 218) all demonstrated that TTBPT is not toxic to sediment bacteria or organisms.

TTBPT is listed as a "Registered Substances Considered Not to Be PBT/vPvB"[12] under the European Union's Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) Regulation 1907/2006. TTBPT is also listed as "low bioconcentration" on Japan's Chemical Substance Control Law (CSCL) List of Examined Existing Chemical Substances.

Authoritative and Screening Lists

- **Authoritative:** None.
- **Screening:** None.

[12] vPvB = Very Persistent and Very Bioaccumulative.

Studies

- **NICNAS (2006):**
  - In a bioaccumulation study performed using test methods for new chemical substances (Kanpogyo No. 5 Yakuhatsu No. 615, 49 Kikyoku No. 392, 1974), red killifish (*Oryzias latipes*) were exposed to nominal concentrations of TTBPT (CAS # 25713-60-4) at 0.5 or 0.05 mg/L for 8 weeks using a continuous flow-through system. Analytical monitoring was performed using HPLC. The BCFs were determined to be <0.8-9 and 8.0-18 for 0.5 and 0.05 mg/L, respectively (Kurume Research Laboratory, 1990b, as cited in NICNAS, 2006). The study authors concluded that TTBPT is "not bioaccumulative in the food chain as the BCF criteria are not exceeded. Further, the notified chemical high molecular weight and low water solubility suggests that it is unlikely to cross biological membranes and bioaccumulate (Connell 1990). Release to the aquatic environment will be very limited from the proposed uses and thus aquatic toxicity is unlikely to occur" (NICNAS, 2006). However, according to ICL-IP Europe B.V. (2017), the "[f]ish were exposed to 0.5 mg/l which is much above the maximum level of water solubility of the substance. Therefore, although no bioconcentration was observed, valid results cannot be derived due to the concentrations used."
- **ICL-IP Europe B.V. (2017) and Huntingdon Life Sciences Ltd. (2006):**
  - In a mammalian oral ADME study (OECD TG 417), Sprague-Dawley rats (n = 12/sex/dose) were administered a single dose of 50 or 1,000 mg/kg-day of radiolabeled TTBPT suspended in 0.5% carboxymethycellulose *via* gastric intubation. The radiolabeled TTBPT was entirely excreted *via* the feces (95.4-105%), with the majority excreted within the interval of 0-48 hours. Very low amounts of radioactivity were found in the urine (0.2%), expired air (<0.1%), carcass (<0.01% of the low dose; 0.03-1.27% of the high dose), and cage washes (0.01-0.26%). The total absorption was estimated to be 0.2% of the administered dose. Based on the study findings, it was concluded that TTBPT is not likely to be absorbed or accumulate in biological tissues.
- **Zheng *et al*. (2022):**
  - The potential metabolism of TTBPT was studied both using *in vitro* systems as well as *via in vivo* administration to rats. The authors reported that when incubated with human and rat liver microsomes, TTBPT was rapidly metabolized, with half-lives of 1.1 and 2.2 hours, respectively. The authors noted that tribromophenol (TBP) would be a potential metabolite of TTBPT. This *in vitro* result is not inconsistent with the results reported above, which indicated that very little TTBPT was absorbed, so metabolite formation *in vivo* would overall be very limited and unlikely to be detected. The authors also administered 250 mg/kg TTBPT to rats for 7 days and then assayed their blood for the presence of TBP. TBP was detected in the blood at a concentration of 270 ± 110 µg/g lipid weight. This can be adjusted by the blood volume and blood lipid content for a rat, estimated at 0.014 g total blood lipids per rat (UCSF, 2020; Noble and Boucek, 1955). This results in 3.8 µg of TBP in the blood after exposure to 250 mg/kg (48 mg per rat, based on reported rat body weights) daily for 7 days. This represents 0.008% of the daily administered dose and suggests that the metabolism of TTBPT to TBP is not significant. Note that Zheng *et al*. (2022) stated that the "average formation rate" of TBP from TTBPT in the blood was 1.3%, but do not provide the basis for this estimate (*e.g*., whether it is relative to the daily or cumulative administered dose or the concentration of the parent chemical in blood). In the ADME study described above, the absorption of TTBPT was found to be about 0.2% of the administered dose. If this estimate is combined with the formation rate of 1.3% given by Zheng *et al*. (2022), it yields a TBP production rate of 0.002% relative to the daily dose of TTBPT, which is similar to the 0.008% production rate derived above.

Physical Hazards (Phys.)

Reactivity (Rx)

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

TTBPT is assigned a score of **Low (L)** for reactivity, with high confidence. This score is based on adequate studies of the oxidizing potential and explosiveness of TTBPT, and is supported by the use of TTBPT as a flame retardant and the fact that the chemical structure of TTBPT does not contain "chemical groups that would infer explosive properties" or "chemical groups that might act as an oxidising agent" (NICNAS, 2006). NICNAS (2006) additionally notes that TTBPT is "expected to be stable under normal use conditions," though it would decompose around 375°C and release potentially poisonous and corrosive fumes (hydrogen bromide, carbon monoxide, carbon dioxide, and nitrogen oxides) (NICNAS, 2006). This score is assigned with high confidence because it is based on experimental data in well-conducted, reliable tests.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **NICNAS (2006):**
  - TTBPT was tested in a series of experiments that assessed explosive/oxidizing properties conducted according to the EC Directive 92/69/EEC A.14 Explosive Properties method and the EC Directive 92/69/EEC A.17 Oxidising Properties (Solids) method. The results of these studies predict that TTBPT has no oxidizing properties and is nonexplosive (NOTOX, 1997g,h, as cited in NICNAS, 2006).

Flammability (F)

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

TTBPT is assigned a score of **Low (L)** for flammability, with high confidence. This score is based on TTBPT's use as a flame retardant and the results of a preliminary screening test.

Authoritative and Screening Lists

- **Authoritative:** Not listed.
- **Screening:** Not listed.

Studies

- **NICNAS (2006):**
  - TTBPT was tested in a preliminary screening test that assessed its flammability and auto-ignition temperature according to the EC Directive 92/69/EEC A.10 Flammability (Solids) method and the 92/69/EEC A.16 Relative Self-Ignition Temperature for Solids method. In terms of flammability, TTBPT emitted orange sparks and black smoke when in contact with the ignition source in a preliminary screening test. However, after the ignition source was removed, the spark extinguished immediately. Thus, no further testing was performed. No self-ignition was observed, and TTBPT melted and turned into a black residue around 400°C. Based on these findings, TTBPT was not considered highly flammable (NOTOX, 1997e,f, as cited in NICNAS, 2006).

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Appendix A

Hazard Endpoint Acronyms

Hazard Endpoint Acronyms

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

PHAROS Results – Chemical Name and Associated Transformation Products

Appendix II

Hazard Export from Pharos for "[118-79-6] 2,4,6-TRIBROMOPHENOL"
https://pharosproject.net/chemicals/2005269
2022-04-22

Hazard Name	List Name	Hazard Inherited From	Endpoint	Hazard Level	GreenScreen List Translator Score	GreenScreen List Type	Pharos Endpoint	Pharos Hazard Level	Pharos Priority	C2C Endpoint	C2C Hazard Level	HPD Priority List
PBT - Chemical for Priority Action	OSPAR - Priority PBTs & EDs & equivalent concern	BROMINATED FLAME RETARDANTS (BFR)	PBT [Persistence, Bioaccumulation, and any of the following: Acute Aquatic Toxicity, Chronic Aquatic Toxicity, Carcinogenicity, Mutagenicity, Reproductive Toxicity, Developmental Toxicity, Systemic Toxicity/Organ Effects repeated exposure]	Unspecified	LT-1	Authoritative A	PBT	Very High	Purple	Multiple Endpoints	Red	Yes
Flame retardant substance class of concern for PB&T & long range transport	EHP - San Antonio Statement on BFRs & CFRs	BROMINATED FLAME RETARDANTS (BFR)	PBT (Persistence, Bioaccumulation & Toxicity)	Very High	NoGS	Not included in GreenScreen	PBT	Very High	Purple			Yes
H361 - Suspected of damaging fertility or the unborn child [Toxic to reproduction - Category 2]	GHS - Japan		Reproductive Toxicity	Moderate	LT-UNK	Screening A	REPRODUCTIVE	Medium	Orange	Reproductive Toxicity (Repro + Dev)	Red	No
Endocrine Disruption	ChemSec - SIN List		Endocrine Activity	High to Moderate	LT-P1	Screening B	ENDOCRINE	Medium	Orange	Endocrine Disruption	Red or Yellow	Yes
Potential Endocrine Disruptor	TEDX - Potential Endocrine Disruptors		Endocrine Activity	High to Moderate	LT-P1	Screening B	ENDOCRINE	Medium	Orange	Endocrine Disruption	Red or Yellow	Yes
UNEP EDCs	UNEP EDCs		Endocrine Activity	Potential Concern	NoGS	Not included in GreenScreen	ENDOCRINE	Potential Concern	Blue			No
Muta. 2; H341 - Suspected of causing genetic defects (modeled)	DK-EPA - Danish Advisory List		Mutagenicity/Genotoxicity	Potential Concern	NoGS	Not included in GreenScreen	GENE MUTATION	Potential Concern	Grey			No
H302 - Harmful if swallowed [Acute Toxicity (oral) - Category 4]	GHS - Japan		Acute Mammalian Toxicity	Moderate	LT-UNK	Screening A	MAMMALIAN	Medium	Yellow	Oral Toxicity	Yellow	No
Acute oral toxicity category 4	GHS - New Zealand		Acute Mammalian Toxicity	Moderate	LT-UNK	Screening A	MAMMALIAN	Medium	Yellow	Oral, Dermal, and/or Inhalative Toxicity		No
Acute Tox. 3 - Toxic if swallowed (modeled)	DK-EPA - Danish Advisory List		Acute Mammalian Toxicity	Potential Concern	NoGS	Not included in GreenScreen	MAMMALIAN	Potential Concern	Grey			No
H319 - Causes serious eye irritation [Serious eye damage / eye irritation - Category 2A]	GHS - Japan		Eye Irritation/Corrosivity	High	LT-UNK	Screening A	EYE IRRITATION	High	Orange	Skin, Eye, and Respiratory Corrosion/Irritation	Yellow	No
H319 - Causes serious eye irritation (unverified) [Serious eye damage/eye irritation - Category 2A]	EU - Manufacturer REACH hazard submissions		Eye Irritation/Corrosivity	Potential Concern	NoGS	Not included in GreenScreen	EYE IRRITATION	Potential Concern	Grey			No
H317 - May cause an allergic skin reaction [Skin sensitizer - Category 1]	GHS - Japan		Skin Sensitization	High	LT-UNK	Screening B	SKIN SENSITIZE	High	Orange	Skin and Respiratory Sensitization	Red	No
H317 - May cause an allergic skin reaction (unverified) [Skin sensitization - Category 1]	EU - Manufacturer REACH hazard submissions		Skin Sensitization	Potential Concern	NoGS	Not included in GreenScreen	SKIN SENSITIZE	Potential Concern	Grey			No
H371 - May cause damage to organs [Specific target organs/systemic toxicity following single exposure - Category 2]	GHS - Japan		Systemic Toxicity/Organ Effects [Single Exposure] and/or Neurotoxicity [Single Exposure]	High	LT-UNK	Screening A	ORGAN TOXICANT	High	Orange	Oral, Dermal, and/or Inhalative Toxicity	Yellow	No
H373 - May cause damage to organs through prolonged or repeated exposure [Specific target organs/systemic toxicity following repeated exposure - Category 2]	GHS - Japan		Systemic Toxicity/Organ Effects [Repeated Exposure] and/or Neurotoxicity [Repeated Exposure]	Moderate	LT-UNK	Screening A	ORGAN TOXICANT	Medium	Yellow	Oral, Dermal, and/or Inhalative Toxicity	Yellow	No
H400 - Very toxic to aquatic life [Hazardous to the aquatic environment (acute) - Category 1]	GHS - Japan		Acute Aquatic Toxicity	Very High	LT-UNK	Screening A	ACUTE AQUATIC	Very High	Orange	Acute Aquatic Toxicity (Fish, Invertibrates, and/or Algae)	Red	No
Aquatic Acute1 - Very toxic to aquatic life (modeled)	DK-EPA - Danish Advisory List		Acute Aquatic Toxicity	Potential Concern	NoGS	Not included in GreenScreen	ACUTE AQUATIC	Potential Concern	Grey			No
Aquatic Chronic1 - Very toxic to aquatic life with long lasting effects (modeled)	DK-EPA - Danish Advisory List		Acute Aquatic Toxicity	Potential Concern	NoGS	Not included in GreenScreen	ACUTE AQUATIC	Potential Concern	Grey			No
H400 - Very toxic to aquatic life (unverified) [Hazardous to the aquatic environment (acute) - Category 1]	EU - Manufacturer REACH hazard submissions		Acute Aquatic Toxicity	Potential Concern	NoGS	Not included in GreenScreen	ACUTE AQUATIC	Potential Concern	Grey			No
H410 - Very toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment (chronic) - Category 1]	GHS - Japan		T & P and/or B [(Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	Unspecified	LT-P1	Screening B	CHRON AQUATIC	Very High	Orange	Chronic Aquatic Toxicity (Fish, Invertibrates, and/or Algae)		No
Flame Retardants	American Apparel and Footwear Association Restricted Substance List (AAFA RSL)	Halogenated Flame Retardants (HFRs)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No

Appendix II

Hazard Name	List Name	Hazard Inherited From	Endpoint	Hazard Level	GreenScreen List Translator Score	GreenScreen List Type	Pharos Endpoint	Pharos Hazard Level	Pharos Priority	C2C Endpoint	C2C Hazard Level	HPD Priority List
Core Restrictions	C2C Certified v4 Product Standard Restricted Substances List (RSL) - Effective July 1, 2021	HALOGENATED ORGANIC COMPOUNDS	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Candidate Chemical List	CA SCP - Candidate Chemicals		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
CoHC List (non SVHC)	CPA - Chemical Footprint	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Substances selected for RMOA or hazard assessment	EU - PACT-RMOA Substances		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Brominated Organic Compounds	GreenScreen Certified Standard for Cleaners & Degreasers RSL	Brominated Organic Compounds	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Organohalogens (including chlorinated plastics)	GreenScreen Certified Standard for Food Service Ware	HALOGENATED ORGANIC COMPOUNDS	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Flame Retardants	GSPI - Six Classes of Problematic Chemicals	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Declarable and Reference Substance Lists (DSL and RSL)	IEC 62474 - Material Declaration for Products of and for the Electrotechnical Industry		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Red List substance to avoid in Living Building Challenge V2.1 projects	Living Building Challenge 2.1 - Red List of Materials & Chemicals	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Prospective Red List substances to avoid in Living Building Challenge projects	Living Building Challenge 3.0 - Red List of Materials & Chemicals	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Red List substances to avoid in Living Building Challenge V3 projects	Living Building Challenge 3.0 - Red List of Materials & Chemicals		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Red List substances to avoid in Living Building Challenge V3.1 projects	Living Building Challenge 3.1 - Red List of Materials & Chemicals		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Red List substances to avoid in Living Building Challenge V4.0 projects	Living Building Challenge 4.0 - Red List of Materials & Chemicals		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Chemicals of High Concern	MDH - Chemicals of High Concern and Priority Chemicals		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Precautionary list of substances recommended for avoidance	P&W - Precautionary List	Halogenated Flame Retardants (HFRs)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Substances of Very High Concern (RIVM ZZS)	Substances of Very High Concern (RIVM ZZS)	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
TSCA Chemical Substance Inventory - Active	TSCA Chemical Substance Inventory (Active-Inactive)		Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Substance to avoid to fulfill LEED Pilot Credit 11	USGBC - LEED Pilot Credits	BROMINATED FLAME RETARDANTS (BFR)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No
Substance to avoid to fulfill LEED Pilot Credit 54 Option 2	USGBC - LEED Pilot Credits	Halogenated Flame Retardants (HFRs)	Restricted List	Potential Concern	NoGS	Not included in GreenScreen	RESTRICTED LIST	Potential Concern	Blue			No

Appendix C

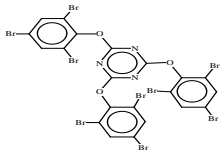
EPI Suite Modeling Results

Appendix II

CAS Number:
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

---------- EPI SUMMARY (v4.11) ----------

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



KOWWIN Program (v1.68) Results:

Log Kow(version 1.68 estimate): 11.46

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	21	Aromatic Carbon	0.2940	6.1740
Frag	3	Aromatic Nitrogen	-0.7324	-2.1972
Frag	9	-Br [bromine, aromatic attach]	0.8900	8.0100
Frag	3	-O- [aliphatic O, two aromatic attach]	0.2923	0.8769
Factor	1	sym-Triazine ring correction	0.8856	0.8856
Factor	3	Ortho-subst on di-aromatic ether (non-cyl)	-0.8396	-2.5188
Const		Equation Constant		0.2290
			Log Kow =	11.4595

MPBPVP (v1.43) Program Results:
Experimental Database Structure Match: no data

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 767.73 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 334.62 deg C (Gold and Ogle Method)
Mean Melt Pt : 342.23 deg C (Joback; Gold,Ogle Methods)
Selected MP: 337.66 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 767.73 deg C (estimated))
(Using MP: 337.66 deg C (estimated))
VP: 2.34E-029 mm Hg (Antoine Method)
: 3.12E-027 Pa (Antoine Method)
VP: 6.97E-019 mm Hg (Modified Grain Method)
: 9.29E-017 Pa (Modified Grain Method)
VP: 3.95E-018 mm Hg (Mackay Method)
: 5.27E-016 Pa (Mackay Method)

```
  Selected VP:  6.97E-019 mm Hg (Modified Grain Method)
             :  9.29E-017 Pa (Modified Grain Method)
  Subcooled liquid VP:  2.48E-015 mm Hg (25 deg C, Mod-Grain method)
                     :  3.31E-013 Pa  (25 deg C, Mod-Grain method)
```

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-O- (nonring)	25.16	75.48
Group	6	CH (aromatic)	28.53	171.18
Group	15	-C (aromatic)	30.76	461.40
Group	3	N (aromatic)	39.88	119.64
Group	9	-Br (to aromat)	61.85	556.65
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		1582.53
RESULT- corr		BOILING POINT in deg Kelvin		1040.89
		BOILING POINT in deg C		767.73

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-O- (nonring)	22.23	66.69
Group	6	CH (aromatic)	8.13	48.78
Group	15	-C (aromatic)	37.02	555.30
Group	3	N (aromatic)	68.40	205.20
Group	9	-Br (to aromat)	43.43	390.87
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		1389.34
RESULT-limit		MELTING POINT in deg Kelvin		623.00
		MELTING POINT in deg C		349.84

```
Water Sol from Kow (WSKOW v1.42) Results:
=========================================

          Water Sol: 1.849e-011 mg/L

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)
         Br
CHEM   :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
---------------------------------- WSKOW v1.42 Results -----------------------
Log Kow  (estimated)  :  11.46
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  11.46

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -16.761
   Water Solubility at 25 deg C (mg/L):  1.849e-011



WATERNT Program (v1.01) Results:
================================
```

Water Sol (v1.01 est): 1.0674e-006 mg/L

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br

CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	Aromatic Carbon (C-H type)	-0.3359	-2.0152
Frag	1	Aromatic Nitrogen [max count of 1 allowed]	1.9255	1.9255
Frag	9	-Br [bromine, aromatic attach]	-0.5661	-5.0953
Frag	3	-O- [aliphatic O, two aromatic attach]	0.3181	0.9542
Frag	15	Aromatic Carbon (C-substituent type)	-0.5400	-8.0993
Const		Equation Constant		0.2492
NOTE		Minimum Solubility (log S = -12.00) Applied!		

Log Water Sol (moles/L) at 25 dec C = -12.0000
Water Solubility (mg/L) at 25 dec C =1.0674e-006

ECOSAR Program (v1.11) Results:
==========
ECOSAR Version 1.11 Results Page

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br

CHEM :
CAS Num:
ChemID1:
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
Log Kow: 11.460 (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: 1.849E-011 (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: 11.460 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 1.849E-011 (mg/L, EPISuite WSKowwin v1.43 Estimate)

ECOSAR v1.11 Class-specific Estimations

Triazines, Aromatic

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Triazines, Aromatic	Fish	96-hr	LC50	4.02e-006 *
Triazines, Aromatic	Daphnid	48-hr	LC50	0.000605 *
Triazines, Aromatic	Green Algae	96-hr	EC50	5.56e-005 *
Triazines, Aromatic	Fish		ChV	1.65e-007 *
Triazines, Aromatic	Daphnid		ChV	1.44e-005 *
Triazines, Aromatic	Green Algae		ChV	0.000463 *
Triazines, Aromatic	Fish (SW)	96-hr	LC50	9.09e-005 *
Triazines, Aromatic	Mysid (SW)	96-hr	LC50	1.05e-005 *

Triazines, Aromatic	: Fish (SW)		ChV	0.000378 *
Triazines, Aromatic	: Mysid (SW)		ChV	7.06e-011 *
Neutral Organic SAR	: Fish	96-hr	LC50	2.8e-006 *
(Baseline Toxicity)	: Daphnid	48-hr	LC50	3.81e-006 *
	: Green Algae	96-hr	EC50	0.000105 *
	: Fish		ChV	7.67e-007 *
	: Daphnid		ChV	4.22e-006 *
	: Green Algae		ChV	0.000192 *

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.

Triazines, Aromatic:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (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)

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 2.42E-012 atm-m3/mole (2.46E-007 Pa-m3/mole)
Group Est: Incomplete

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

HENRYWIN v3.20 Results

CLASS		BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6	Hydrogen to Carbon (aromatic) Bonds		-0.9258
FRAGMENT	18	Car-Car		4.7485
FRAGMENT	9	Car-Br		2.2084
FRAGMENT	6	Car-Nar		9.7693
FRAGMENT	6	Car-O		2.0836
FACTOR	2	Additional aromatic nitrogen(s)		-5.0000
FACTOR	3	-O-carbon ortho-position to Nar		-2.8800
RESULT		BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	10.004

HENRYs LAW CONSTANT at 25 deg C = 2.42E-012 atm-m3/mole
= 9.91E-011 unitless
= 2.46E-007 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	6 Car-H (Car)(Car)		0.66
	9 Car (Car)(Car)(Br)		4.41
	3 Car (Car)(Car)(O)		-1.29
	3 Nar (Car)(Car)		9.18
	3 O (Car)(Car)	ESTIMATE	5.10
	MISSING Value for: Car (Nar)(Nar)(O)		
	MISSING Value for: Car (Nar)(O)(Nar)		
	MISSING Value for: Car (Nar)(O)(Nar)		
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	INCOMPLETE	18.06

For Henry LC Comparison Purposes:
  Exper Database: none available
  User-Entered Henry LC: not entered
  Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
    HLC: 5.294E-008 atm-m3/mole (5.364E-003 Pa-m3/mole)
    VP: 6.97E-019 mm Hg (source: MPBPVP)
    WS: 1.85E-011 mg/L (source: WSKOWWIN)

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 21.465

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 21.465
Koa (octanol/air) estimate: 2.915e+021
Using:
  Log Kow: 11.46 (KowWin est)
  HenryLC: 2.42e-012 atm-m3/mole (HenryWin est)
  Log Kaw: -10.005 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 11.46 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 2.42e-012 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 21.465 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:
==========
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
---------- BIOWIN v4.10 Results ----------

  Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
  Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
  Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant
  Biowin4 (Primary Biodegradation Timeframe): Recalcitrant
  Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast

Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	0.0095	0.0095
Frag	9	Aromatic bromide [-Br]	-0.1103	-0.9931
Frag	3	Aromatic ether [-O-aromatic carbon]	0.1319	0.3957
MolWt	*	Molecular Weight Parameter		-0.5082
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-0.3484

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	-5.7252	-5.7252
Frag	9	Aromatic bromide [-Br]	-1.6779	-15.1011
Frag	3	Aromatic ether [-O-aromatic carbon]	2.2483	6.7449
MolWt	*	Molecular Weight Parameter		-15.1576
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	-0.2459	-0.2459
Frag	9	Aromatic bromide [-Br]	-0.1360	-1.2240
Frag	3	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.1744
MolWt	*	Molecular Weight Parameter		-2.3589
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		-0.8039

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	-0.0575	-0.0575
Frag	9	Aromatic bromide [-Br]	-0.1535	-1.3816
Frag	3	Aromatic ether [-O-aromatic carbon]	0.0771	0.2314
MolWt	*	Molecular Weight Parameter		-1.5400
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		1.0999

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	0.1168	0.1168
Frag	9	Aromatic bromide [-Br]	0.1668	1.5010
Frag	3	Aromatic ether [-O-aromatic carbon]	0.1952	0.5857
Frag	6	Aromatic-H	0.0082	0.0493
MolWt	*	Molecular Weight Parameter		-3.1756
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.2107

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	-9.3006	-9.3006
Frag	9	Aromatic bromide [-Br]	1.5021	13.5192
Frag	3	Aromatic ether [-O-aromatic carbon]	1.3227	3.9681
Frag	6	Aromatic-H	0.1201	0.7208
MolWt	*	Molecular Weight Parameter		-30.8155
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Triazine ring (symmetric)	-0.0783	-0.0783
Frag	9	Aromatic bromide [-Br]	0.0000	0.0000
Frag	3	Aromatic ether [-O-aromatic carbon]	0.1780	0.5340
Frag	6	Aromatic-H	-0.0954	-0.5726
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.7193

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

BioHCwin (v1.01) Program Results:

SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br
CHEM :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44

BioHCwin v1.01 Results

NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 3.31E-013 Pa (2.48E-015 mm Hg)
Log Koa (Koawin est): 21.465
Kp (particle/gas partition coef. (m3/ug)):

```
      Mackay model           :  9.07E+006
      Octanol/air (Koa) model:  7.16E+008
   Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  1
      Mackay model           :  1
      Octanol/air (Koa) model:  1


AOP Program (v1.92) Results:
============================
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)
         Br
CHEM   :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction       =   0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings =   1.4807 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =   1.4807 E-12 cm3/molecule-sec
   HALF-LIFE =     7.224 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =    86.684 Hrs
.......................  ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
Fraction sorbed to airborne particulates (phi):
  1 (Junge-Pankow, Mackay avg)
  1 (Koa method)
     Note: the sorbed fraction may be resistant to atmospheric oxidation



KOCWIN Program (v2.00) Results:
===============================
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)
         Br
CHEM   :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
---------------------------  KOCWIN v2.00 Results  --------------------------

  Koc Estimate from MCI:
  ----------------------
        First Order Molecular Connectivity Index  ........... : 16.994
        Non-Corrected Log Koc (0.5213 MCI + 0.60)  .......... :  9.4588
        Fragment Correction(s):
                 2   Ether, aromatic  (-C-O-C-)  ...........  : -1.3582
                 1   Triazine  ring  .......................  : -0.2257
        Corrected Log Koc  ................................. :  7.8750

                           Estimated Koc:  7.499e+007  L/kg   <===========

  Koc Estimate from Log Kow:
  --------------------------
        Log Kow  (Kowwin estimate)  ......................... : 11.46
        Non-Corrected Log Koc (0.55313 logKow + 0.9251)  .... :  7.2640
        Fragment Correction(s):
                 2   Ether, aromatic  (-C-O-C-)  ...........  :  0.1118
                 1   Triazine  ring  .......................  : -0.1239
```

```
        Corrected Log Koc  ..................................  :  7.2519

                        Estimated Koc:  1.786e+007  L/kg   <==========



HYDROWIN Program (v2.00) Results:
================================
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br)
         Br
CHEM   :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
--------------------------- HYDROWIN v2.00 Results ---------------------------


 Currently, this program can NOT estimate a hydrolysis rate constant for
                the type of chemical structure entered!!

 ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
      Specific Alkyl Halides & Phosphorus Esters can be estimated!!

   When present, various hydrolyzable compound-types will be identified.
  For more information, (Click OVERVIEW in Help  or  see the User's Guide)

              *****   CALCULATION NOT PERFORMED   *****



BCFBAF Program (v3.01) Results:
==============================
SMILES : c1c(cc(c(c1Br)Oc2nc(nc(n2)Oc3c(cc(cc3Br)Br)Br)Oc4c(cc(cc4Br)Br)Br)Br)
         Br
CHEM   :
MOL FOR: C21 H6 Br9 N3 O3
MOL WT : 1067.44
-------------------------------- BCFBAF v3.01 --------------------------------
Summary Results:
  Log BCF (regression-based estimate):  1.42   (BCF = 26.4 L/kg wet-wt)
  Biotransformation Half-Life (days) :  812  (normalized to 10 g fish)
  Log BAF (Arnot-Gobas upper trophic):  3.94   (BAF = 8.77e+003 L/kg wet-wt)

Log Kow (experimental):  not available from database
Log Kow used by BCF estimates:  11.46

Equation Used to Make BCF estimate:
   Log BCF = -0.49 log Kow + 7.554 + Correction

      Correction(s):                    Value
       Aromatic sym-triazine ring      -0.517

   Estimated Log BCF =  1.422  (BCF = 26.42 L/kg wet-wt)

=========================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
=========================================================
------+-----+-------------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Triazine ring (symmetric)                | -0.0123 | -0.0123
 Frag |  9  |  Aromatic bromide   [-Br]                 |  0.3964 |  3.5672
 Frag |  3  |  Aromatic ether  [-O-aromatic carbon]     | -0.0694 | -0.2082
 Frag |  6  |  Aromatic-H                               |  0.2664 |  1.5983
 Frag |  3  |  Benzene                                  | -0.4277 | -1.2832
 L Kow|  *  |  Log Kow =  11.46 (KowWin estimate)       |  0.3073 |  3.5220
 MolWt|  *  |  Molecular Weight Parameter               |         | -2.7373
 Const|  *  |  Equation Constant                        |         | -1.5371
```

RESULT	LOG Bio Half-Life (days)	2.9095
RESULT	Bio Half-Life (days)	811.9
NOTE	Bio Half-Life Normalized to 10 g fish at 15 deg C	

Biotransformation Rate Constant:
 kM (Rate Constant): 0.0008538 /day (10 gram fish)
 kM (Rate Constant): 0.0004801 /day (100 gram fish)
 kM (Rate Constant): 0.00027 /day (1 kg fish)
 kM (Rate Constant): 0.0001518 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
   Estimated Log BCF (upper trophic) = 0.451 (BCF = 2.827 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 3.943 (BAF = 8772 L/kg wet-wt)
   Estimated Log BCF (mid trophic) = 0.577 (BCF = 3.777 L/kg wet-wt)
   Estimated Log BAF (mid trophic) = 3.585 (BAF = 3842 L/kg wet-wt)
   Estimated Log BCF (lower trophic) = 0.617 (BCF = 4.142 L/kg wet-wt)
   Estimated Log BAF (lower trophic) = 3.313 (BAF = 2056 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
   Estimated Log BCF (upper trophic) = 0.585 (BCF = 3.845 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 4.176 (BAF = 1.501e+004 L/kg wet-wt)

Volatilization From Water

Chemical Name:

Molecular Weight : 1067.40 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 2.42E-012 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	7.904E+008	8.623E+009
HALF-LIFE (days) :	3.293E+007	3.593E+008
HALF-LIFE (years) :	9.017E+004	9.837E+005

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using 10000 hr Bio P,A,S)

PROPERTIES OF:

Molecular weight (g/mol)	1067.4
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	2.42E-012
Air-water partition coefficient	9.89708E-011
Octanol-water partition coefficient (Kow)	2.88403E+011
Log Kow	11.46
Biomass to water partition coefficient	5.76806E+010
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	10000.00	10000.00
-Aeration tank	0.00	10000.00	10000.00

```
         -Settling tank       0.00     10000.00       10000.00

 STP Overall Chemical Mass Balance:
 ----------------------------------
                              g/h               mol/h          percent

Influent                    1.00E+001         9.4E-003        100.00

Primary sludge              5.99E+000         5.6E-003        59.89
Waste sludge                3.34E+000         3.1E-003        33.36
Primary volatilization      1.14E-016         1.1E-019         0.00
Settling volatilization     2.52E-016         2.4E-019         0.00
Aeration off gas            6.22E-016         5.8E-019         0.00

Primary biodegradation      1.75E-002         1.6E-005         0.18
Settling biodegradation     4.26E-003         4.0E-006         0.04
Aeration biodegradation     5.61E-002         5.3E-005         0.56

Final water effluent        5.96E-001         5.6E-004         5.96

Total removal               9.40E+000         8.8E-003        94.04
Total biodegradation        7.79E-002         7.3E-005         0.78


Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   :
  Molecular Wt: 1067.4
  Henry's LC  : 2.42e-012 atm-m3/mole (Henrywin program)
  Vapor Press : 6.97e-019 mm Hg  (Mpbpwin program)
  Liquid VP   : 8.62e-016 mm Hg  (super-cooled)
  Melting Pt  : 338 deg C (Mpbpwin program)
  Log Kow     : 11.5  (Kowwin program)
  Soil Koc    : 7.5e+007  (KOCWIN MCI method)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.105          173          1000
   Water     4.17           4.32e+003    1000
   Soil      92.9           8.64e+003    1000
   Sediment  2.79           3.89e+004    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       4.98e-021    90.8        227         3.03        7.58
   Water     7.04e-022    145         903         4.83        30.1
   Soil      1.41e-021    1.61e+003   0           53.7        0
   Sediment  1.9e-021     10.8        12.1        0.359       0.403

   Persistence Time: 7.21e+003 hr
   Reaction Time:    1.16e+004 hr
   Advection Time:   1.89e+004 hr
   Percent Reacted:  61.9
   Percent Advected: 38.1

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      173.4
      Water:    4320
      Soil:     8640
      Sediment: 3.888e+004
        Biowin estimate: -0.804  (recalcitrant)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Appendix D

OECD QSAR Toolbox Version 4.4.1 Results

Documents

Document 1

[C: 1;Md: 0;P: 0] CAS: 25713604

Profiling methods

Options 1 Selected

Filter endpoint tree...

1 [target]

Structure

- Structure info
- Parameters
- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
- Profiling
  - Endpoint Specific
    - Respiratory sensitisation

No alert found