

## **GreenScreen® Assessment for [Polyphosphonate (CAS#68664-06-2)]**

**Method Version: GreenScreen® Version 1.2<sup>1</sup>**

**Verified or Non-Verified<sup>2</sup>: NON-VERIFIED**

### **Introduction<sup>3,4,5</sup>**

This GreenScreen assessment is based on the information reported in the corresponding chemical hazard profile in “An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report”<sup>3</sup>. Additional information on hazard endpoints beyond what was included in the final report was not sought with the exception of reactivity. Hazard classification information for reactivity was supplemented because it is not included in the DfE report but is needed to apply the GreenScreen Benchmark system.

Hazard classification levels reported in the DfE profiles and in this GreenScreen report may differ due to differences between criteria as defined in the DfE “Alternatives Assessment Criteria for Hazard Evaluation”<sup>4</sup> and the GreenScreen for Safer Chemicals v1.2 methods<sup>5</sup>. Any differences in interpretation are explained and justified in this GreenScreen report.

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Licensed Profiler or Certified Practitioner (specify): N/A	

**Confirm application of the *Disclosure and Assessment Rules and Best Practice*<sup>6</sup>:** (List any deviations)

Disclosure thresholds applied by DfE are unclear in the DfE report.

**Chemical Name (CAS #):**

<sup>1</sup> Use GreenScreen® Assessment Procedure (Guidance) V1.2

<sup>2</sup> “NON-VERIFIED” means that Verification Has Not Been Performed on this GreenScreen Assessment

<sup>3</sup> An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report Available at: <http://www.epa.gov/dfe/pubs/projects/decaBDE/deca-report-complete.pdf>, p 4-539, accessed 2/9/2014.

<sup>4</sup> Available at: [http://www.epa.gov/dfe/alternatives\\_assessment\\_criteria\\_for\\_hazard\\_eval.pdf](http://www.epa.gov/dfe/alternatives_assessment_criteria_for_hazard_eval.pdf), accessed 10/2013.

<sup>5</sup> Details available at: <http://www.cleanproduction.org/Greenscreen.v1-2.php>, accessed 10/2013.

<sup>6</sup> See GreenScreen Guidance V1.2 Section 8

## Polyphosphonate (CAS#68664-06-2)

### Also Called:

Phosphonic acid, P-methyl-, diphenyl ester, polymer with 4,4'-(1-methylethylidene)bis[phenol]

### Tradenames:

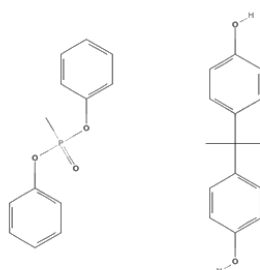
FRX 100 (polyphosphonate) (Polymeric additive); FRX100

### Suitable analogs or moieties of chemicals used in this assessment (CAS #'s):

No analog

### Chemical Structure(s):

\*Note: Include chemical structure(s) of all suitable analogs (and /or moieties) used in the assessment.



### Notes related to production specific attributes<sup>7</sup>:

#### For Inorganic Chemicals and relevant particulate organics (if not relevant, list NA)

##### Define Properties:

1. Particle size (e.g., silica of respirable size)
2. Structure (e.g., amorphous vs. crystalline)
3. Mobility (e.g., water solubility, volatility)
4. Bioavailability: No absorption is expected for any route of exposure for polyphosphonate. This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.

#### For Polymeric Materials: (delete this section if not a polymeric material)

According to DfE, "This alternative is a high MW polymer with <1% low (<1,000) MW oligomers. The high MW oligomers, with a MW >1,000, are assessed together using the professional judgment and information contained in the literature concerning polymer assessment (Boethling et al., 1997)."

The polymer is produced from the condensation of methyldiphenylphosphonate and bisphenol A equivalents. The MW of polyphosphonate ranges between 10,000 and 50,000. Oligomers with MW <1,000 are expected to be present at <1% in the polyphosphonate mixture. Phenoxy terminated oligomers are anticipated to predominate."<sup>8</sup>

<sup>7</sup> Note any composition or hazard attributes of the chemical product relevant to how it is manufactured. For example, certain synthetic pathways or processes result in typical contaminants, by-products or transformation products. Explain any differences between the manufactured chemical product and the GreenScreen assessment of the generic chemical by CAS #.

<sup>8</sup> An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report Available at: <http://www.epa.gov/dfe/pubs/projects/decaBDE/deca-report-complete.pdf>, p 4-539, accessed 2/9/2014.

### Identify Monomers and Corresponding Properties

1. % of Each Monomer
  - a) Monomer 1
  - b) Monomer 2
  - c) Monomer 3
2. Are the monomers blocked? (Y/N)
3. Molecular Weight (MW) of polymeric material: The MW of polyphosphonate ranges between 10,000 and 50,000.
4. % of polymeric material with
  - a) MW <500
  - b) MW <1,000: Oligomers with MW <1,000 are expected to be present at <1% in the polyphosphonate mixture.
5. % Weight Residual Monomers
6. Solubility/Dispersability/Swellability
7. Particle size
8. Overall charge of polymeric material
9. Identify constituents and residual concentrations of
  - a) Catalysts
  - b) Processing aids
10. Identify any monomers, oligomers, catalysts or processing aids classified as Benchmark 1 according to the hazard identification lists in the GreenScreen List Translator.

### Identify Applications/Functional Uses:

(e.g., Cleaning product, TV casing)

1. Flame Retardant

### GreenScreen Benchmark Score and Hazard Summary Table:<sup>9,10,11,12</sup>

[Polyphosphonate was assigned a **Benchmark Score of 3** based on very high persistence. Polyphosphonate could be a Benchmark 2 if the data gap endocrine activity or respiratory sensitization was filled with data indicating a moderate hazard score.

Green Screen Hazard Ratings: [Polyphosphonate]																			
Group I Human					Group II and II* Human								Ecotox		Fate		Physical		
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	L	L	L	DG	L		L*		L	L	DG	L	L	L	L	vH	vL	L	L

<sup>9</sup> See Appendix A for a glossary of hazard endpoint acronyms

<sup>10</sup> See Appendix B for alternative GreenScreen Hazard Summary Table (Classification presented by exposure route)

<sup>11</sup> For inorganic chemicals only, see GreenScreen Guidance V1.2 Section 14.4. (Exceptions for Persistence)

<sup>12</sup> For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen Guidance V1.2 Section 9.3.

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

\*While DfE assigned a moderate score for repeat dose toxicity due to possibility of lung overloading as a result of dust forming operations, it has been concluded that this is not a likely exposure scenario based on identified uses and therefore has not been included in the GreenScreen assessment.

### Environmental Transformation Products and Ratings<sup>13</sup>:

**Identify feasible and relevant environmental transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern<sup>14</sup>**

Functional Use	Life Cycle Stage	Transformation Pathway	Environmental Transformation Products	CAS #	Feasible and Relevant?	GreenScreen List Translator Score or GreenScreen Benchmark Score
			None			

### Hazard Classification Summary Section:

#### For all hazard endpoints:

- Search all GreenScreen specified lists. Report relevant results either in each hazard endpoint section or attach to the end of the report.
- Always indicate if suitable analogs or models were used.
- Attach modeling results (See Appendix C).
- Include all references either in each hazard endpoint section or at the end of the report.

### Group I Human Health Effects (Group I Human)

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

Polyphosphonate was assigned a score of LOW for Carcinogenicity based on a low score within the EPA's DfE alternatives assessment. The low designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in *italics* within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

**LOW:** This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive

<sup>13</sup> See GreenScreen Guidance V1.2 Section 13

<sup>14</sup> 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.

functional groups, inhalation potential and hindered amine groups are not expected. Therefore, there is low potential for carcinogenicity.

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

Polyphosphonate was assigned a score of LOW for Mutagenicity based on a low score within the EPA's DfE alternatives assessment. The low designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.

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

Polyphosphonate was assigned a score of LOW for Reproductive Toxicity based on a low score within the EPA's DfE alternatives assessment. For reproductive toxicity, EPA's DfE uses numerical data quantifying the hazard associated with the 3 different hazard levels, whereas Green-Screen does not base the hazard score on a numerical rating system but bases classifications on listing under GHS, the EU and NTP. Therefore the conversion of DfE's developmental and reproductive toxicity conclusions to comparable GreenScreen hazard scores is done on a case by case basis. DfE's low score was based on expert judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.

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

Polyphosphonate was assigned a score of LOW for Developmental Toxicity based on a low score within the EPA's DfE alternatives assessment. For developmental toxicity, EPA's DfE uses numerical data quantifying the hazard associated with the 3 different hazard levels, whereas Green-Screen does not base the hazard score on a numerical rating system but bases classifications on listing under GHS, the EU and NTP. Therefore the conversion of DfE's developmental and reproductive toxicity conclusions to comparable GreenScreen hazard scores is done on a case by case basis. DfE's low score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:

LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.

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

Polyphosphonate was assigned a score of DATA GAP for Endocrine Activity. This conclusion was made based on no data located.

No data located. This polymer is large, with a MW >1,000. Based on professional judgment, polyphosphonate is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.

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

*Note: Group II and Group II\* endpoints are distinguished in the v 1.2 Benchmark system (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**

Polyphosphonate was assigned a score of LOW for Acute Mammalian Toxicity. The low designation for Acute Mammalian Toxicity in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on empirical data and expert judgment within EPA's alternatives assessment and therefore is not reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:  
LOW: Based on experimental LD<sub>50</sub> values > 2,000 mg/kg. This compound is also expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.

#### **Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)**

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

DfE evaluates Systemic Toxicity based on repeated exposures. Lack of data for Systemic Toxicity based on a single exposure does not constitute a data gap when data for repeated exposures are available.

##### **(ST-repeat) Group II\* Score (repeated dose: H, M, L): L**

Polyphosphonate was assigned a score of LOW for Systemic Toxicity/Organ Effects based on repeated exposure. The low designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The low designation within EPA's alternatives assessment is based on expert judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:  
LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the MW<sub>n</sub> is >10,000, there is the possibility of lung overloading if >5% of the particles are in the respirable range as a result of dust forming operations.

In addition:

Based on professional judgment polyphosphonate is expected to have limited bioavailability and therefore is of low concern.

#### **Neurotoxicity (N)**

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

DfE evaluates Neurotoxicity based on repeated exposures. Lack of data for Neurotoxicity based on a single exposure does not constitute a data gap when data for repeated exposures are available.

##### **(N-repeat) Group II\* Score (repeated dose: H, M, L): L**

Polyphosphonate was assigned a score of LOW for Neurotoxicity based on a low score within the EPA's DfE alternatives assessment. This conclusion was based on expert judgment due to limited bioavailability. The low designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.

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

Polyphosphonate was assigned a score of LOW for Skin Sensitization. This conclusion was based on analogy to other high MW polymers with similar structural features. The low designation for skin sensitization in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on professional judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:

LOW: Based on expert judgment, polyphosphonate is estimated not to have potential for skin sensitization

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

Polyphosphonate was assigned a score of DATA GAP for Respiratory Sensitization. This conclusion was made based on no data located.

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

Polyphosphonate was assigned a score of LOW for Skin Irritation/Corrosivity based on expert judgment. The low designation for skin irritation in the EPA's alternatives assessment corresponds to a moderate hazard in GreenScreen. However the data presented in the DfE report indicates this compound is a low irritation hazard. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: Based on expert judgment, polyphosphonate is estimated to not have potential for dermal irritation. (This summary seems more consistent with DfE VERY LOW criteria.)

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

Polyphosphonate was assigned a score of LOW for Eye Irritation based upon expert judgment within the EPA's DfE alternatives assessment. The low designation for eye irritation in the EPA's alternatives assessment corresponds to a moderate hazard in GreenScreen. However the data presented in the DfE report indicates this compound is a low irritation hazard. The score was based on expert judgment by analogy to other high MW polymers with similar structural features and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: Based on expert judgment, polyphosphonate is estimated to not have potential for eye irritation. (This summary seems more consistent with DfE VERY LOW criteria.)

**Ecotoxicity (Ecotox)**

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

Polyphosphonate was assigned a score of LOW for Acute Aquatic Toxicity. The low designation for acute aquatic toxicity in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to have no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to its large size.

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

Polyphosphonate was assigned a score of LOW for Chronic Aquatic Toxicity. The low designation for chronic aquatic toxicity in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on professional judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:

LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to its large size.

**Environmental Fate (Fate)**

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

Polyphosphonate was assigned a score of VERY HIGH for Persistence. The very high designation for persistence in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:

VERY HIGH: This polymer is large, with a MW>1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. The polymer does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths. Evaluation of these degradation values suggest a half-life of >180 days.

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

Polyphosphonate was assigned a score of VERY LOW for Bioaccumulation. The low designation for bioaccumulation in EPA's alternatives assessment is equivalent to a very low score in GreenScreen. The score was based on professional judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was summarized as follows:



LOW: This polymer is large, with a MW >1,000. It is expected to have poor bioavailability indicating that this polymer should be of low potential for bioaccumulation.

### **Physical Hazards (Physical)**

#### **Reactivity (Rx) Score (vH, H, M or L): *L***

Polyphosphonate was assigned a score of LOW for Reactivity based on professional judgment and structural similarity to other chemicals. Because of the lack of concrete data for this endpoint, the score of LOW was italicized.

Very little information is publicly available on the reactivity of polyphosphonate. It is, however, a co-polymer of two other chemicals that have undergone extensive review. The phosphate monomer is similar to phosphate containing flame retardants such as triphenylphosphate (TPP) which is currently used extensively in consumer products and has been found not to be reactive. Bisphenol A is used extensive in polycarbonate plastic and polycarbonate based flame retardants. These two chemicals will be used as a surrogate for reactivity of the polymer as the polymer is less likely to be as reactive as these monomers.

The National Library of Medicine's Hazardous Substances Database indicates that TPP has an NFPA Hazard Classification of '0' for instability and that it is '*...normally stable, even under fire exposure conditions, and that do not react with water.*'

The European Commission in a IUCLID dataset indicated that Bisphenol A is only explosive when '*... in powder or granular form, mixed with air.*' The European Union states in its Risk Assessment Report that '*Bisphenol A is not explosive in the conventional sense or when considering structure or chemical groupings.*' and '*Bisphenol A is not an oxidising agent on the basis of structural considerations.*'

Based upon professional judgment and the information above, polyphosphonate is unlikely to be reactive.

#### **References:**

National Library of Medicine Hazardous Substances Database, available at:  
<http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~dinA2S:1>, accessed 12/2013.

European Commission, European Chemicals Bureau, IUCLID Dataset, 2/19/2000, 114 p., available at: [http://esis.jrc.ec.europa.eu/doc/IUCLID/data\\_sheets/80057.pdf](http://esis.jrc.ec.europa.eu/doc/IUCLID/data_sheets/80057.pdf), accessed 12/2013.

European Union Risk Assessment Report on 4,4'-Isopropylidenediphenol (Bisphenol A), February 20120, 270 pages, available at:  
[http://esis.jrc.ec.europa.eu/doc/risk\\_assessment/REPORT/bisphenolareport325.pdf](http://esis.jrc.ec.europa.eu/doc/risk_assessment/REPORT/bisphenolareport325.pdf), access 12/2013.

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

Polyphosphonate was assigned a score of LOW for Flammability based on a not flammable description within the DfE report. This conclusion was based on adequate data and is not reported in italics.

**APPENDIX A: Hazard Benchmark Acronyms  
(alphabetical order)**

- (AA) Acute Aquatic Toxicity**
- (AT) Acute Mammalian Toxicity**
- (B) Bioaccumulation**
- (C) Carcinogenicity**
- (CA) Chronic Aquatic Toxicity**
- (Cr) Corrosion/ Irritation (Skin/ Eye)**
- (D) Developmental Toxicity**
- (E) Endocrine Activity**
- (F) Flammability**
- (IrE) Eye Irritation/Corrosivity**
- (IrS) Skin Irritation/Corrosivity**
- (M) Mutagenicity and Genotoxicity**
- (N) Neurotoxicity**
- (P) Persistence**
- (R) Reproductive Toxicity**
- (Rx) Reactivity**
- (SnS) Sensitization- Skin**
- (SnR) Sensitization- Respiratory**
- (ST) Systemic/Organ Toxicity**