



United States
Environmental Protection Agency

Office of Chemical Safety
and Pollution Prevention

Final Risk Evaluation for Cyclic Aliphatic Bromide Cluster (HBCD)

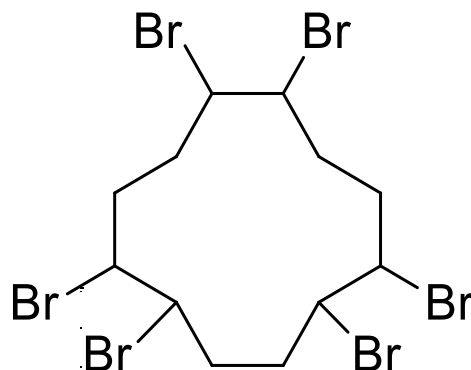
Systematic Review Supplemental File:

Data Quality Evaluation of Physical-Chemical Properties Studies

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Table of Contents

Table 1. Physical Form Study Summary for HBCD	3
Table 2. Melting Point Study Summary for HBCD.....	4
Table 3. Boiling Point Study Summary for HBCD	5
Table 4. Density Study Summary for HBCD	6
Table 5. Vapor Pressure Study Summary for HBCD.....	7
Table 6. Water Solubility Study Summary for HBCD	8
Table 7. Octanol-water Partition Coefficient Study Summary for HBCD.....	9
Table 8. Henry's Law Constant Study Summary for HBCD.....	10
Table 9. Autoflammability Temperature Study Summary for HBCD.....	11

Table 1. Physical Form Study Summary for HBCD

Study Reference:	<p>EINECS (2008). Risk assessment: HBCD. CAS No.: 25637-99-4. Luxembourg European Inventory of Existing Chemical Substances, Office for Official Publicants of the European Communities. https://echa.europa.eu/documents/10162/661bff17-dc0a-4475-9758-40bdd6198f82. HERO ID: 1443914</p>		
Note:	EINECS (2008) reported the physical form of HBCD.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The information was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The information is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	High	The information is from a secondary source that was written by experts and is widely available for public review.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	Not rated	Data source does not provide information to determine the method objectivity (unbiased method). Thus, the domain/metric was not rated.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Not rated	This metric is not applicable to this type of information.
Overall Quality Level			High

Table 2. Melting Point Study Summary for HBCD

Study Reference:	<p>EINECS (2008). Risk assessment: HBCD. Cas No.: 25637-99-4. Luxembourg European Inventory of Existing Chemical Substances, Office for Official Publicants of the European Communities. https://echa.europa.eu/documents/10162/661bff17-dc0a-4475-9758-40bdd6198f82. HERO ID: 1443914</p>		
Note:	<p>EINECS (2008) cited Smith et al. 2005 (HERO ID 787904) who reported the melting point of HBCD.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest. The results reported in the secondary source (EINECS) are ranges that extend beyond what was measured in Smith et al. (2005).
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	High	The value is reported in a secondary source which was prepared by experts and cited to a peer-reviewed journal article as the original source.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	Methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	Data are obtained by accepted standard analytic methods.
Overall Quality Level			High

Table 3. Boiling Point Study Summary for HBCD

Study Reference:	<p>Peled, M; Scharia, R; Sondack, D. (1995). Thermal rearrangement of hexabromo-cyclododecane (HBCD). In: Advances in organobromine chemistry II. Elsevier. New York, NY. HERO ID: 3421461</p>		
Note:	<p>Peled et al. (2005) reported the boiling point of HBCD.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value was consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	High	The value is reported in a secondary source which was prepared by experts and cited to a peer-reviewed journal article as the original source.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	Methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	Data are obtained by accepted standard analytic methods.
Overall Quality Level			High

Table 4. Density Study Summary for HBCD

Study Reference:	<p>EINECS (2008). Risk assessment: HBCD. Cas No.: 25637-99-4. Luxembourg European Inventory of Existing Chemical Substances, Office for Official Publicants of the European Communities. https://echa.europa.eu/documents/10162/661bff17-dc0a-4475-9758-40bdd6198f82. HERO ID: 1443914</p>		
Note:	EINECS (2008) who reported the density of HBCD.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value was consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	Medium	The value is reported in a secondary source which was prepared and reviewed by experts; however, it is cited to a chemical corporation with unknown reliability and review.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	Low	The secondary source describes the method as non-GLP.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			Medium

Table 5. Vapor Pressure Study Summary for HBCD

Study Reference:	<p>Stenzel and Nixon (1997). Determination of the vapor pressure using a spinning rotor gauge. 1997; 439C-117, pp 44. Wildlife international Ltd., Easton, Maryland. HERO ID: 3588056</p>		
Note:	<p>Stenzel and Nixon (1997) reported the vapor pressure of HBCD.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	Medium	From a source that is not described as High but is known.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The method reported is designed to answer a specific question.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Medium	The method used is not recommended for this chemical according to OECD guideline 104; however, the authors considered this value acceptable since similar values were reported by another source using a different method.
Overall Quality Level			High

Table 6. Water Solubility Study Summary for HBCD

Study Reference:	<p>EINECS (2008). Risk assessment: HBCD. Cas No.: 25637-99-4. Luxembourg European Inventory of Existing Chemical Substances, Office for Official Publicants of the European Communities. https://echa.europa.eu/documents/10162/661bff17-dc0a-4475-9758-40bdd6198f82. HERO ID: 1443914</p>		
Note:	<p>EINECS (2008) cites MacGregor and Nixon (1997) who reported the water solubility of HBCD.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	Medium	The value is reported in a secondary source which was prepared and reviewed by experts; however, the original source is a report with unknown review or reliability.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology as described by the secondary source is designed to answer a specific question.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The analytical method used, as described by the secondary source, is an accepted standard method.
Overall Quality Level			High

Table 7. Octanol-water Partition Coefficient Study Summary for HBCD

Study Reference:	MacGregor and Nixon (1997). Hexabromocyclododecane (HBCD): Determination of n-octanol/water partition coefficient with cover letter dated 06/27/1997. HERO ID: 787767		
Note:	MacGregor and Nixon (1997) reported the octanol-water partition coefficient of HBCD.		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	Medium	From a source that is not described as High but is known.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology as described by the secondary source is designed to answer a specific question.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The analytical method used, as described by the secondary source, is an accepted standard method.
Overall Quality Level			High

Table 8. Henry's Law Constant Study Summary for HBCD

Study Reference:	<p>U.S. EPA. (2012b). Estimation Programs Interface Suite for Microsoft Windows, v. 4.11. https://www.epa.gov/tsca-screening-tools/download-epi-suite-estimation-program-interface-v411. HERO ID: 2347246</p>		
Note:	<p>The Henry's Law constant was calculated by EPI Suite™ using measured water solubility and vapor pressure data.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The Henry's Law constant has been calculated using measured water solubility and vapor pressure data for the compound of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The water solubility and vapor pressure values used to determine the Henry's Law constant were from reliable sources and the derivation method has been shown to accurately match measured values.
Evaluation/Review	The information or data reported has reliable review.	High	The water solubility and vapor pressure values used to derive the Henry's Law constant are from reliable sources that are peer-reviewed and available to the public. The derivation method has also been peer-reviewed.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The method for producing this value is not biased towards a particular outcome.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Low	The analytical methods used to determine the water solubility and vapor pressure values used in the Henry's Law constant derivation are not reported.
Overall Quality Level			High

Table 9. Autoflammability Temperature Study Summary for HBCD

Study Reference:	<p>EINECS (2008). Risk assessment: HBCD. Cas No.: 25637-99-4. Luxembourg European Inventory of Existing Chemical Substances, Office for Official Publicants of the European Communities. https://echa.europa.eu/documents/10162/661bff17-dc0a-4475-9758-40bdd6198f82. HERO ID: 1443914</p>		
Note:	<p>EINECS (2008) stated that decomposition of HBCD occurs before an autoflammability temperature is reached. Therefore, the confidence in the decomposition temperature of the boiling point study by Peled et al. (2005; HERO ID 3421461) is also evaluated here.</p>		
Domain/Metric	Description/ Definition	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comment
Representativeness	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The value was consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	High	The value is reported in a secondary source which was prepared by experts and cited to a peer-reviewed journal article as the original source.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	Not rated	The value is reported in a secondary source and does not provide information to determine the method objectivity (unbiased method). Thus, the domain/metric was not rated.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	Low	The value is reported in a secondary and does not provide information regarding the analytical method.
Overall Quality Level			High