

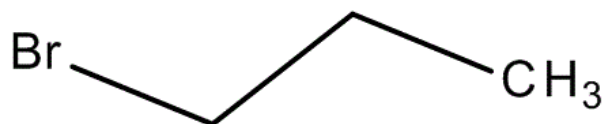


**Final Risk Evaluation for  
1-Bromopropane  
(*n*-Propyl Bromide)**

**Systematic Review Supplemental File:**

**Data Quality Evaluation of Physical-Chemical Properties Studies**

**CASRN: 106-94-5**



*August 2020*

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Table 1. Physical Form Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <b>The Merck index: An encyclopedia of chemicals, drugs, and biologicals.</b> In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. <b>HERO ID: 3378176</b>		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the physical form is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	Information was reported for the subject chemical substance.
<b>Appropriateness</b>	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.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Not rated	This metric is not applicable to this type of information.
<b>Overall Quality Level</b>			<b>High</b>

Table 2. Melting Point Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <b>The Merck index: An encyclopedia of chemicals, drugs, and biologicals.</b> In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. <b>HERO ID: 3378176</b>		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the melting point is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 3. Boiling Point Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <i>The Merck index: An encyclopedia of chemicals, drugs, and biologicals</i> . In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. <b>HERO ID: 3378176</b>		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the boiling point is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 4. Density Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <i>The Merck index: An encyclopedia of chemicals, drugs, and biologicals</i> . In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. HERO ID: 3378176		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the density is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 5. Vapor Pressure Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<b>Boublík, T; Fried, V; Hála, E. (1984). The vapour pressures of pure substances: Selected values of the temperature dependence of the vapour pressures of some pure substances in the normal and low pressure region (2nd Revised ed.). Amsterdam, The Netherlands: Elsevier Science Publishers. HERO ID: 194873</b>		
<b>Note:</b>	Boublik et al. (1984) reported the vapor pressure of 1-bromopropane.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection in which results have been selected by experts based on their quality and availability. References to the original sources are included.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 6. Vapor Density Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<b>Patty, F. A., et al., Eds. (1963). Industrial Hygiene and Toxicology: Vol. II: Toxicology. New York, NY, Interscience Publishers. HERO ID: 2329543</b>		
<b>Note:</b>	The primary source was unavailable; therefore, the data quality evaluation for the vapor density was performed on the secondary source (HSDB citing Patty et al., 1963).		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	Value is reported for the subject chemical substance.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Reported value is consistent with the chemical substance structure.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	Medium	Value is included in a data collection that is widely available to the public and cites original sources.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>Medium</b>



Table 7. Water Solubility Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<p>Yalkowsky, SH; He, Y; Jain, P. (2010). <b>Handbook of aqueous solubility data</b> (2nd ed.). Boca Raton, FL: CRC Press.  <a href="http://dx.doi.org/10.1201/EBK1439802458">http://dx.doi.org/10.1201/EBK1439802458</a>.  <b>HERO ID: 2990992</b></p>		
<b>Note:</b>	<p>Yalkowsky et al. (2010) reported the water solubility of 1-bromopropane.</p>		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use. Original sources are also referenced.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 8. Octanol-water Partition Coefficient Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<b>Hansch, C. (1995). Fundamentals and applications in chemistry and biology - hydrophobic, electronic and steric constants. In Exploring QSAR. Washington DC: American Chemical Society Professional Reference Book/Oxford University Press. HERO ID: 2991086</b>		
<b>Note:</b>	Hansch (1995) reported the Log K <sub>OW</sub> of 1-bromopropane.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection that has been compiled by experts and includes references to the original sources. The original source for this value is a peer-reviewed journal.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 9. Henry's Law Constant Study Summary for 1-Bromopropane

Study Reference:	<p>U.S. EPA. (2012b). Estimation Programs Interface Suite for Microsoft Windows, v. 4.11. <a href="https://www.epa.gov/tsca-screening-tools/download-epi-suite-estimation-program-interface-v411">https://www.epa.gov/tsca-screening-tools/download-epi-suite-estimation-program-interface-v411</a>.                  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.
<b>Overall Quality Level</b>			<b>High</b>

Table 10. Flash Point Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <i>The Merck index: An encyclopedia of chemicals, drugs, and biologicals</i> . In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. HERO ID: 3378176		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the flash point is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 11. Autoflammability Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<b>NFPA. (2010). Fire protection guide to hazardous materials (14th ed.). Quincy, MA. HERO ID: 2991057</b>		
<b>Note:</b>	NFPA reported the autoflammability for 1-bromopropane. The confidence of the data has been evaluated using the 13th edition (2002) since the 14th edition was unavailable, and the data value was unchanged.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	Medium	The value was reported in a known data collection that has been available to the public and was compiled using data from reliable sources. Original sources are not reported (although they are available upon request) and peer-review has not been performed; therefore, this metric has been rated medium.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	High	The value was obtained by an accepted analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 12. Viscosity Study Summary for 1-Bromopropane

<b>Study Reference:</b>	Haynes, WM; Lide, DR. (2010). Editor CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data (91st ed.). Boca Raton, FL: CRC Press. HERO ID: 2192464		
<b>Note:</b>	Haynes and Lide (2010) reported the viscosity of 1-bromopropane.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 13. Refractive Index Study Summary for 1-Bromopropane

<b>Study Reference:</b>	O'Neil, MJ. (2013). <i>The Merck index: An encyclopedia of chemicals, drugs, and biologicals</i> . In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry. HERO ID: 3378176		
<b>Note:</b>	O'Neil (2013) reported various physical-chemical properties and only the confidence of the refractive index is evaluated.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>

Table 14. Dielectric Constant Study Summary for 1-Bromopropane

<b>Study Reference:</b>	<b>Haynes, WM; Lide, DR. (2010). Editor CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data (91st ed.). Boca Raton, FL: CRC Press. HERO ID: 2192464</b>		
<b>Note:</b>	Haynes and Lide (2010) reported the dielectric constant of 1-bromopropane.		
<b>Domain/Metric</b>	<b>Description/ Definition</b>	<b>Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]</b>	<b>Comment</b>
<b>Representativeness</b>	The information or data reflects the data and chemical substance type.	High	The data was measured for the substance of interest.
<b>Appropriateness</b>	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	The measured value is consistent with the nature of the substance.
<b>Evaluation/Review</b>	The information or data reported has reliable review.	High	The information is from a recognized data collection where data are peer-reviewed by experts in the field and are broadly available to the public for review and use.
<b>Reliability/ Unbiased (Method Objectivity)</b>	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.
<b>Reliability/ Analytic Method</b>	The information or data reported is from a reliable method.	Low	Data source does not provide information regarding the analytical method.
<b>Overall Quality Level</b>			<b>High</b>