Final Risk Evaluation for
1,4-Dioxane

Systematic Review Supplemental File:

Data Quality Evaluation of Physical-Chemical Properties Studies

CASRN: 123-91-1
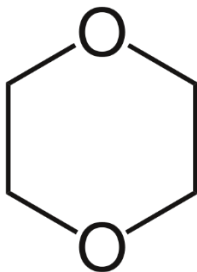
December 2020

This document is a compilation of tables for the data extraction and evaluation for 1,4-Dioxane. Each table shows the data point or set or information element that was extracted and evaluated from a data source in accordance with Appendix D of the *Application of Systematic Review in TSCA Risk Evaluations*. If the source contains more than one data set or information element, the review provides an overall confidence score for each data set or information element that is found in the source. Therefore, it is possible that a source may have more than one overall quality/ confidence score.

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Table 1. Molecular Weight Study Summary for 1,4-Dioxane

Study Reference:	**Haynes WM et al. (2014). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. 95th ed. CRC Press, Boca Raton, FL.** **HERO ID: 2828348**
Note:	Haynes et al. (2014). reported various physical-chemical properties and only the confidence of the molecular weight is evaluated.

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 measured value is consistent with the nature of the substance.
Evaluation/Review	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.
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. Physical Form Study Summary for 1,4-Dioxane

Study Reference:	**O'Neil, M.J., ed. (2001). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 14th ed., Whitehouse Station, NJ: Merck and Co., Inc., p. 581.** **HERO ID: 595055**		
Note:	O'Neil (2001) reported various physical-chemical properties and only the confidence of the physical form is evaluated.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	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.
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 3. Melting Point Study Summary for 1,4-Dioxane

Study Reference:	**Haynes WM et al. (2014). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. 95th ed. CRC Press, Boca Raton, FL.** **HERO ID: 2828348**
Note:	Haynes et al. (2014). reported various physical-chemical properties and only the confidence of the melting point is evaluated.

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 measured value is consistent with the nature of the substance.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 4. Boiling Point Study Summary for 1,4-Dioxane

Study Reference:	**O'Neil, M.J., ed. (2006). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 14th ed., Whitehouse Station, NJ: Merck and Co., Inc., p. 1054.** **HERO ID: 737461**		
Note:	O'Neil (2006) reported various physical-chemical properties and only the confidence of the boiling point is evaluated.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 5. Density Study Summary for 1,4-Dioxane

Study Reference:	O'Neil, M.J., ed. (2001). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 14th ed., Whitehouse Station, NJ: Merck and Co., Inc., p. 581. HERO ID: 595055		
Note:	O'Neil (2001) reported various physical-chemical properties and only the confidence of the density is evaluated.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 6. Vapor Pressure Study Summary for 1,4-Dioxane

Study Reference:	**Lewis RJ, Sr. (1999). Sax's dangerous properties of industrial materials. New York, NY: John Wiley & Sons.** **HERO ID: 625540**		
Note:	Lewis (1999) reported the vapor pressure.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	The information or data reported has reliable review.	High	The information or data is from a recognized data collection
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 7. Vapor Density Study Summary for 1,4-Dioxane

Study Reference:	**Lewis R.J Sr. (2012). Sax's dangerous properties of industrial materials. New York, NY: John Wiley & Sons.** **HERO ID: 3840105**		
Note:	Lewis (2012) reported the vapor density.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	The information or data reported has reliable review.	High	The information or data is from a recognized data collection.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 8. Water Solubility Study Summary for 1,4-Dioxane

Study Reference:	**Yalkowsky, SH; He, Y; Jain, P. (2010). Handbook of aqueous solubility data (2nd ed.). Boca Raton, FL: CRC Press.** **http://dx.doi.org/10.1201/EBK1439802458.** **HERO ID: 2990992**
Note:	Yalkowsky et al. (2010) reported the water solubility.

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 measured value is consistent with the nature of the substance.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 9. Octanol-water Partition Coefficient Study Summary for 1,4-Dioxane

Study Reference:	Hansch, C., Leo, A., D. Hoekman. (1995). Exploring QSAR – Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society. HERO ID: 51424		
Note:	Hansch et al. (1995) reported the log Kow.		
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 measured value is consistent with the nature of the substance.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 10. Henry's Law Constant Study Summary for 1,4-Dioxane

Study Reference:	**Park, J. H., et al. (1987). Experimental reexamination of selected partition coefficients from Rohrschneider's data set. Analytical Chemistry 59(15): 1970-1976.** **HERO ID: 194328**		
Note:	Park et al. (1987) reported the Henry's Law Constant.		
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	Data presented for the subject chemical substance.
Appropriateness	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.
Evaluation/Review	The information or data reported has reliable review.	High	The value was from a peer-reviewed 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 analytic methods.
Overall Quality Level			**High**

Table 11. Flash Point Study Summary for 1,4-Dioxane

Study Reference:	Larranaga, MD; Lewis, RJ; Lewis, RA (Eds.) (2016) In Hawley's condensed chemical dictionary (16th, pp. 512). Hoboken, NJ: John Wiley & Sons, Inc. HERO ID: 5333260		
Note:	Larranaga et al. (2016) reported the flash point.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	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.
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.	High	Data are obtained by accepted standard analytic methods.
Overall Quality Level			High

Table 12. Autoflammability Study Summary for 1,4-Dioxane

Study Reference:	USCG, (1999). Chemical Hazards Response Information System (CHRIS) Hazardous Chemical Data. Washington, DC. HERO ID: 5208492		
Note:	USCG (1999) reported the autoflammability temperature.		
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 measured value is consistent with the nature of the substance.
Evaluation/Review	The information or data reported has reliable review.	High	The information is from a recognized data collection.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 13. Viscosity Study Summary for 1,4-Dioxane

Study Reference:	O'Neil, M.J., ed. (2013). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 15th ed., Whitehouse Station, NJ: Merck and Co., Inc. HERO ID: 3378176		
Note:	O'Neil (2013) reported various physical-chemical properties and only the viscosity is evaluated.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			High

Table 14. Refractive Index Study Summary for 1,4-Dioxane

Study Reference:	**Haynes WM et al. (2014). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. 95th ed. CRC Press, Boca Raton, FL.** **HERO ID: 2828348**		
Note:	Haynes et al. (2014) reported various physical-chemical properties and only the refractive index is evaluated.		
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 measured value is consistent with the nature of the substance.
Evaluation/Review	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.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**

Table 15. Dielectric Constant Study Summary for 1,4-Dioxane

Study Reference:	**Bruno, T. J. and P. D. N. Svoronos (2006). CRC Handbook of Fundamental Spectroscopic Correlation Charts. Boca Raton, FL, CRC Press.** **HERO ID: 3839962**		
Note:	Haynes et al. (2014) reported various physical-chemical properties and only the refractive index is evaluated.		
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	Data presented for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data cited as found in the literature.
Evaluation/Review	The information or data reported has reliable review.	High	The information is from a recognized data collection.
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.	Low	Data source does not provide information regarding the analytical method.
Overall Quality Level			**High**