United States
Environmental Protection Agency

Office of Chemical Safety and
Pollution Prevention

Final Risk Evaluation for n-Methylpyrrolidone

Systematic Review Supplemental File:

Data Quality Evaluation of Physical and Chemical Properties Studies

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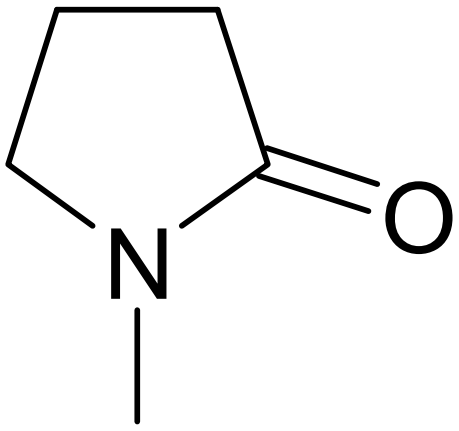

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EPA's Office of Pollution Prevention and Toxics (OPPT) developed data quality criteria for physical and chemical properties studies. The criteria are documented in the *Application of Systematic Review in TSCA Risk Evaluations* document (EPA Document#740-P1-8001).

This systematic review supplemental document describes the data quality evaluation results for physical and chemical properties studies evaluated for the NMP Risk Evaluation.

Table 1. Physical Form Study Summary for N-Methyl-2-pyrrolidone

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 several 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	The information is measured for the subject chemical substance.
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 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. Melting Point Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**Ashford, R.D. (1994) Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., p. 595. HERO ID: 1443889**		
Note:	Ashford (1994) reported the melting point of N-Methyl-2-pyrrolidone.		
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 subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data are consistent with the nature of the subject chemical substance.
Evaluation/Review	The information or data reported has reliable review.	Medium	The data is from a known data collection reference book.
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	Analytical method details are not provided.
Overall Quality Level:			**Medium**

Table 3. Boiling Point Study Summary for N-Methyl-2-pyrrolidone

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 several 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	The data is measured 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	Analytical method details are not provided.
Overall Quality Level:			**High**

Table 4. Density Study Summary for N-Methyl-2-pyrrolidone

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 multiple physical-chemical properties. The confidence of the density is evaluated here.		
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 was measured for the subject chemical substance.
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 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	Analytical method details are not provided.
Overall Quality Level:			**High**

Table 5. Vapor Pressure Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**Daubert, T.E., R.P. Danner. 1989. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis.** **HERO ID: 3827242**		
Note:	Daubert and Danner (1989) reported a regression equation for the vapor pressure of N-Methyl-2-pyrrolidone.		
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 are measured for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Measured data are consistent with the subject chemical substance structural features.
Evaluation/Review	The information or data reported has reliable review.	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use and include references to the original sources.
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.	Low	Underlying experimental studies used to derive the coefficients were cited but analytical details were not provided.
Overall Quality Level:			**High**

Table 6. Vapor Density Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**NFPA. (1997). Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, p. 325-72. HERO ID: 3827456**		
Note:	NFPA (1997) reported the vapor density of N-Methyl-2-pyrrolidone. Data quality evaluation based on the 13th ed. (2002), p 325-89.		
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 is measured for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Data are representative and deemed suitable for general use.
Evaluation/Review	The information or data reported has reliable review.	Medium	Data reported from numerous authoritative sources as well as from manufacturers.
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	Analytical method details are not provided.
Overall Quality Level:			**Medium**

Table 7. Water Solubility Study Summary for N-Methyl-2-pyrrolidone

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 several physical-chemical properties and only the confidence of the water solubility 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 are measured for the subject chemical substance.
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 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	Analytical method details are not provided.
Overall Quality Level:			**High**

Table 8. Octanol-water Partition Coefficient Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**Sasaki, H; Kojima, M; Mori, Y; Nakamura J; Shibasaki, J. (1988). Enhancing effect of pyrrolidone derivatives on transdermal drug delivery I. Int J Pharm, 44, 15–24.** **HERO ID: 3827461**		
Note:	Sasaki H (1988) reported the octanol-water partition coefficient of N-Methyl-2-pyrrolidone.		
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 are measured for the subject chemical substance.
Appropriateness	The information or data reflects anticipated results based on chemical structural features or behaviors.	High	Measured data are consistent with the subject chemical substance structural features.
Evaluation/Review	The information or data reported has reliable review.	High	The data is from a peer-reviewed journal article.
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 9. Henry's Law Constant Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**Kim, BR; Kalis, EM; Dewulf, T; Andrews, KM. (2000). Henry's Law Constant for Paint Solvents and their Implications on Volatile Organic Compound Emissions from Automotive Painting. Water Environ Res 72: 65-74.** **HERO ID: 3578170**		
Note:	Kim et al., (2000) reported the Henry's Law constant of N-Methyl-2-pyrrolidone.		
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 subject chemical substance.
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 peer-reviewed journal article.
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	Values were obtained by accepted standard analytical methods.
Overall Quality Level:			**High**

Table 10. Flash Point Study Summary for N-Methyl-2-pyrrolidone

Study Reference:	**Riddick JA et al., (1986) Techniques of organic chemistry: Organic solvents: Physical properties and methods of purification. 4th ed., Vol 2 p. 666.** **HERO ID: 3827465**		
Note:	Riddick et al., (1986) reported the flash point of N-Methyl-2-pyrrolidone.		
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 was measured for the subject chemical substance.
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 that is reviewed by experts, is widely available to the public, and cites original sources.
Reliability/Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	Medium	The method used to produce the information is designed to answer a specific question.
Reliability/Analytic Method	The information or data reported is from a reliable method.	High	The value was obtained using an accepted standard method.
Overall Quality Level:			**High**

Table 11. Viscosity Study Summary for N-Methyl-2-pyrrolidone

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 multiple physical-chemical properties. The confidence of the viscosity is evaluated here.		
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 was measured for the subject chemical substance.
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 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	Analytical method details are not provided.
Overall Quality Level:			**Medium**