United States
Environmental Protection Agency

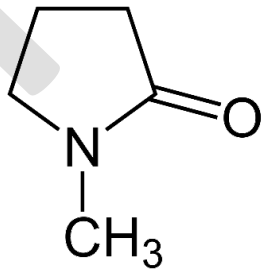
Office of Chemical Safety and
Pollution Prevention

Draft Risk Evaluation for N-Methyl-2-pyrrolidone

Systematic Review Supplemental File:

Data Quality Evaluation of Physical-Chemical Properties Studies

CASRN: 872-50-4



October 2019

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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**

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 NMP.		
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:			**High**

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**

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**

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 NMP.		
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**

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 NMP. 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:			**High**

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**

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 NMP.		
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**

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 NMP.		
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**

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 NMP.		
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**

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:			**High**

EPI Suite™ Model Outputs

CAS Number: 000872-50-4
SMILES : O=C1CCCN1C
CHEM : N-METHYLPYRROLIDONE
MOL FOR: C5 H9 N1 O1
MOL WT : 99.13
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): -0.38
Boiling Point (deg C) : 202.00
Melting Point (deg C) : -25.00
Vapor Pressure (mm Hg) : 0.345
Water Solubility (mg/L): 1E+006
Henry LC (atm-m3/mole) : 3.2E-009

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = -0.11
Log Kow (Exper. database match) = -0.38
Exper. Ref: SASAKI,H ET AL. (1988)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 201.93 (Adapted Stein & Brown method)
Melting Pt (deg C): 25.87 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.326 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C) : 43.5 (Mean VP of Antoine & Grain methods)
MP (exp database): -24 deg C
BP (exp database): 202 deg C
VP (exp database): 3.45E-01 mm Hg (4.60E+001 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 5.53e+005
log Kow used: -0.38 (user entered)
melt pt used: -25.00 deg C
Water Sol (Exper. database match) = 1e+006 mg/L (25 deg C)
Exper. Ref: RIDDICK,JA ET AL. (1986)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 4.5016e+005 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Amides

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 3.16E-008 atm-m3/mole (3.20E-003 Pa-m3/mole)
Group Method: Incomplete
Exper Database: 3.20E-09 atm-m3/mole (3.24E-004 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: 3.200E-009 atm-m3/mole (3.242E-004 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.500E-008 atm-m3/mole (4.560E-003 Pa-m3/mole)
VP: 0.345 mm Hg (source: User-Entered)
WS: 1E+006 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -0.38 (user entered)
Log Kaw used: -6.883 (user entered)
Log Koa (KOAWIN v1.10 estimate): 6.503
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.9105
Biowin2 (Non-Linear Model) : 0.9865
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.9259 (weeks)
Biowin4 (Primary Survey Model) : 3.9101 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.5101
Biowin6 (MITI Non-Linear Model): 0.6426
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -0.1714
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 46 Pa (0.345 mm Hg)
Log Koa (Koawin est): 6.503
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 6.52E-008
Octanol/air (Koa) model: 7.82E-007
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 2.36E-006
Mackay model : 5.22E-006

Octanol/air (Koa) model: 6.25E-005

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 21.9910 E-12 cm3/molecule-sec
Half-Life = 0.486 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 5.837 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
3.79E-006 (Junge-Pankow, Mackay avg)
6.25E-005 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 7.401 L/kg (MCI method)
Log Koc: 0.869 (MCI method)
Koc : 4.651 L/kg (Kow method)
Log Koc: 0.668 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.9694 days (HL = 0.01073 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.043 (BCF = 0.9064)
Log BAF Arnot-Gobas method (upper trophic) = -0.043 (BAF = 0.9064)
log Kow used: -0.38 (user entered)

Volatilization from Water:
Henry LC: 3.2E-009 atm-m3/mole (entered by user)
Half-Life from Model River: 1.822E+005 hours (7590 days)
Half-Life from Model Lake : 1.987E+006 hours (8.281E+004 days)

Removal In Wastewater Treatment:
Total removal: 1.85 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.76 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.066	11.7	1000
Water	32.5	360	1000
Soil	67.3	720	1000
Sediment	0.0697	3.24e+003	0

Persistence Time: 608 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.066	11.7	1000
Water	32.5	360	1000
water	(32.5)		
biota	(6.78e-007)		
suspended sediment	(0.000361)		
Soil	67.3	720	1000
Sediment	0.0697	3.24e+003	0

Persistence Time: 608 hr

Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0716	11.7	1000
Water	39.2	360	1000
water	(39.2)		
biota	(8.17e-007)		
suspended sediment	(1.01e-005)		
Soil	60.6	720	1000
Sediment	0.072	3.24e+003	0

Persistence Time: 562 hr