

Office of Chemical Safety and Pollution Prevention

Draft Risk Evaluation for Methylene Chloride

Systematic Review Supplemental File:

Data Quality Evaluation of Physical-Chemical Properties Studies

CASRN: 75-09-2

CI

October 2019

Table of Contents

Table 1. Physical Form Study Summary for Methylene Chloride	3
Table 2. Melting Point Study Summary for Methylene Chloride	4
Table 3. Boiling Point Study Summary for Methylene Chloride	[
Table 4. Density Study Summary for Methylene Chloride	6
Table 5. Vapor Pressure Study Summary for Methylene Chloride	7
Table 6. Vapor Density Study Summary for Methylene Chloride	8
Table 7. Water Solubility Study Summary for Methylene Chloride	9
Table 8. Octanol-water Partition Coefficient Study Summary for Methylene Chloride	1(
Table 9. Henry's Law Constant Study Summary for Methylene Chloride	.11
Table 10. Viscosity Study Summary for Methylene Chloride	.12
Table 11. Refractive Index Study Summary for Methylene Chloride	13
Table 12. Dielectric Constant Study Summary for Methylene Chloride	14

Table 1. Physical Form Study Summary for Methylene Chloride

Study Reference:	U.S. Coast Guard (1984). CHRIS hazardous chemical data. U.S. Department of Transportation. Washington, DC.		
Note:	U.S. Coast Guard (1984) reported the physical form of methylene chloride.		
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 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.	Medium	The data collection is from a known source that lists several reliable primary sources in its references. However; individual values are not cited to their original sources.
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 information type.
Or	verall Quality Level		High

Table 2. Melting Point Study Summary for Methylene Chloride

Table 2. Melting Point Study Summary for Methylene Chloride			
O'Neil, MJ. (2013). The Merck index: An encyclopedia of chemicals, drugs, and biologicals. In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry.			
Note:	O'Neil (2013) reported confidence of the melt		chemical properties and only the ated.
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.
O	verall Quality Level		High

Table 3. Boiling Point Study Summary for Methylene Chloride

Study Reference: O'Neil, MJ. (2013). The Merck index: An encyclopedia of chemicals, drugs, and biologicals. In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry.				
Note:		O'Neil (2013) 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	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.	
Ov	verall Quality Level		High	

Table 4. Density Study Summary for Methylene Chloride

O'Neil, MJ. (2013). The Merck index: An encyclopedia of chemicals, drugs,			
Study Reference:	and biologicals. In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry.		
Note:	O'Neil (2013) reported confidence of the dens		chemical properties and only the
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.
0	verall Quality Level		High

Table 5. Vapor Pressure Study Summary for Methylene Chloride

Table 5. Vapor Fres	Table 5. Vapor Pressure Study Summary for Methylene Chloride			
Study Reference:	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.			
Note:	Boublik et al. (1984) r	eported the vapor	pressure of methylene chloride.	
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 value was derived by interpolation from a peer-reviewed set of measured vapor pressures (Std. Dev. = 0.09 mm Hg).	
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 data set has been cited to its original source which is peer-reviewed. The authors also state that the quality of the experimental data was considered before its inclusion in the 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.	
O	verall Quality Level		High	

Table 6. Vapor Density Study Summary for Methylene Chloride

Study Reference:	Holbrook, MT. (2003). Methylene chloride. In: Kirk-Othmer Encyclopedia of Chemical Technology. John Wiley & Sons, Inc.		
Note:	Holbrook (2003) reported the vapor density of methylene chloride.		
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 in which results have been selected by experts based on their quality and availability. References to the original sources are included.
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.
0	verall Quality Level		High

Table 7. Water Solubility Study Summary for Methylene Chloride

Study Reference:	Horvath, AL. (1982). Halogenated hydrocarbons: solubility-miscibility in water. Marcel Dekker, Inc. New York, New York.		
Note:	Horvath (1982) reported the water solubility of methylene chloride.		
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 consistency of the value with data measured for other similar chemicals was considered before its inclusion in the data collection.
Evaluation/ Review	The information or data reported has reliable review.	High	The value is from a data collection where data were peer-reviewed, cited to original sources, and had their experimental quality examined before inclusion.
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 the data is not biased towards a particular outcome.
Reliability/ Analytic Method	The information or data reported is from a reliable method.	High	The data collection only includes values that have been obtained using reliable and accepted analytical methods.
O	verall Quality Level		High

Table 8. Octanol-water Partition Coefficient Study Summary for Methylene Chloride

Table 8. Octanol-water Partition Coefficient Study Summary for Methylene Chloride			
Study Reference:	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.		
Note:	Hansch (1995) reporte	d the Log K _{OW} of	methylene chloride.
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.
Ov	verall Quality Level		High

Table 9. Henry's Law Constant Study Summary for Methylene Chloride

Study Reference:	Leighton, DT; Calo, JM. (1981). Distribution coefficients of chlorinated hydrocarbons in dilute air-water systems for groundwater contamination applications.		
Note:	Leighton and Calo (19 value and it has been c		Henry's Law constant as a dimensionless n ³ /mol.
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 value was measured 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 source 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.	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.	High	The analytical method used to measure this value is an accepted standard method.
Overall Quality Level		High	

Table 10. Viscosity Study Summary for Methylene Chloride

Study Reference:	Rossberg, M., Lendle, W., Pfleiderer, A., Togel, A. (2011). Chloromethanes. In: Ullmann's Encyclopedia of Industrial Chemicals. Wiley-VCH Verlag GmbH & Co.		
Note:	Rossberg et al. (2011)	reported the visco	sity of methylene chloride.
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 value 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 was similar to measured values for chemicals of similar structure.
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.	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.
0	verall Quality Level	High	

Table 11. Refractive Index Study Summary for Methylene Chloride

Table 11. Refractive index Study Summary for Methylene Chloride			
Study Reference:	O'Neil, MJ. (2013). The Merck index: An encyclopedia of chemicals, drugs, and biologicals. In MJ O'Neil (Ed.), (15th ed.). Cambridge, UK: Royal Society of Chemistry.		
Note:	O'Neil (2013) reported confidence of the refra		chemical properties and only the luated.
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.
O	verall Quality Level		High

Table 12. Dielectric Constant Study Summary for Methylene Chloride

Study Reference:	Laurence et al. (1994). The empirical treatment of solvent-solute interactions: 15 years of pi*. J Phys Chem 98: 5807-5816.		
Note:	Laurence et al. (1994) reported the dielectric constant of methylene chloride.		
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 value 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 similar to those measured for structurally similar compounds.
Evaluation/ Review	The information or data reported has reliable review.	High	The information is from a peer-reviewed journal.
Reliability/ Unbiased (Method Objectivity)	The method for producing the data/information is not biased towards a particular product or outcome.	High	The methodology for producing 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 by an accepted standard analytical method.
Overall Quality Level			High