United States
Environmental Protection Agency

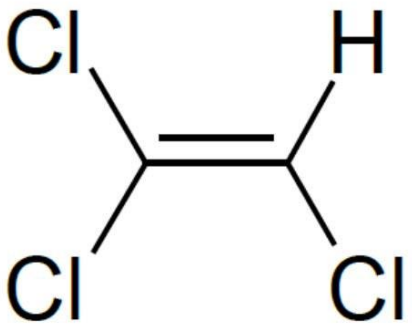
Office of Chemical Safety and
Pollution Prevention

Draft Risk Evaluation for Trichloroethylene

Systematic Review Supplemental File:

Data Quality Evaluation of Physical-Chemical Properties Studies

CASRN: 79-01-6



February 2020

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Table 1. Physical Form Study Summary for Trichloroethylene

Study Reference:	**O'Neil, MJ; Heckelman, PE; Koch, CB. (2006). The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals (14th ed.). Whitehouse Station, NJ: Merck & Co.** **HERO ID: 737461**		
Note:	O'Neil (2006) 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	The information was reported for the substance of interest.
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 Trichloroethylene

Study Reference:	**Lide, DR. (2007). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. In DR Lide (Ed.), (88th ed.). Boca Raton, FL: CRC Press.** **HERO ID: 3827361**		
Note:	Lide (2007) 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 3. Boiling Point Study Summary for Trichloroethylene

Study Reference:	**Lide, DR. (2007). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. In DR Lide (Ed.), (88th ed.). Boca Raton, FL: CRC Press.** **HERO ID: 3827361**		
Note:	Lide (2007) 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.
Overall Quality Level			**High**

Table 4. Density Study Summary for Trichloroethylene

Study Reference:	**ECB. (2000). IUCLID dataset: CAS No. 79-01-6: Trichloroethylene. Ispra, Italy: European Chemicals Bureau, European Commission. Retrieved from https://echa.europa.eu/substance-information/-/substanceinfo/100.001.062. HERO ID: 3809495**		
Note:	ECB (2000) cited Leduc Chemie B.V. (1998) who reported the density of trichlorethylene.		
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.	Medium	The value is reported in a secondary source which was prepared and reviewed by experts; however, the original source is a report with unknown review or reliability.
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			**Medium**

Table 5. Vapor Pressure Study Summary for Trichloroethylene

Study Reference:	**Daubert, TE; Danner, RP. (1989). Physical and thermodynamic properties of pure chemicals: Data compilation. Washington, DC: Taylor & Francis. HERO ID: 194705**		
Note:	Daubert and Danner (1989) reported a regression equation for the vapor pressure of trichloroethylene.		
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	Measured data are consistent with the subject chemical substance structural features.
Evaluation/Review	The information or data reported has reliable review.	High	The information 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 Trichloroethylene

Study Reference:	**O'Neil, MJ; Heckelman, PE; Koch, CB. (2006). The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals (14th ed.). Whitehouse Station, NJ: Merck & Co.** **HERO ID: 737461**		
Note:	O'Neil (2006) reported various physical-chemical properties and only the confidence of the vapor 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	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 7. Water Solubility Study Summary for Trichloroethylene

Study Reference:	**Horvath, AL; Getzen, FW; Maczynska, Z. (1999). IUPAC-NIST Solubility Data Series 67: Halogenated Ethanes and Ethenes with Water. J Phys Chem Ref Data 28: 395-627.** **HERO ID: 729645**		
Note:	Horvath et al. (1999) reported water solubilities at various temperatures for trichloroethylene using a regression-equation based on multiple measured values.		
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	Measured data are consistent with the subject chemical substance structural features.
Evaluation/Review	The information or data reported has reliable review.	High	The information 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 includes 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 8. Octanol-water Partition Coefficient Study Summary for Trichloroethylene

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 9. Henry's Law Constant Study Summary for Trichloroethylene

Study Reference:	**Leighton, DT; Calo, JM. (1981). Distribution coefficients of chlorinated hydrocarbons in dilute air-water systems for groundwater contamination applications.** **HERO ID: 194928**		
Note:	Leighton and Calo (1981) reported the Henry's Law constant as a dimensionless value and it has been converted to atm-m^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. Flash Point Study Summary for Trichloroethylene

Study Reference:	**ECB. (2000). IUCLID dataset: CAS No. 79-01-6: Trichloroethylene. Ispra, Italy: European Chemicals Bureau, European Commission. Retrieved from https://echa.europa.eu/substance-information/-/substanceinfo/100.001.062. HERO ID: 3809495**		
Note:	ECB (2000) cited Petrasol B.V. (1990) who reported the flash point of trichloroethylene.		
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.	Low	There is conflicting data available that indicates this substance is non-flammable.
Evaluation/Review	The information or data reported has reliable review.	Medium	The value is reported in a secondary source which was prepared and reviewed by experts; however, the original source is a report with unknown review or reliability.
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	The analytical method is an accepted standard method.
Overall Quality Level			**Medium**

Table 11. Auto flammability Study Summary for Trichloroethylene

Study Reference:	**ECB. (2000). IUCLID dataset: CAS No. 79-01-6: Trichloroethylene. Ispra, Italy: European Chemicals Bureau, European Commission. Retrieved from https://echa.europa.eu/substance-information/-/substanceinfo/100.001.062. HERO ID: 3809495**		
Note:	ECB (2000) reported the autoflammability temperature of trichloroethylene.		
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.	Medium	The value is reported in a secondary source which was prepared and reviewed by experts; however, the original source is a report with unknown review or reliability.
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			**Medium**

Table 12. Viscosity Study Summary for Trichloroethylene

Study Reference:	**Lide, DR. (2007). CRC handbook of chemistry and physics: A ready-reference book of chemical and physical data. In DR Lide (Ed.), (88th ed.). Boca Raton, FL: CRC Press.** **HERO ID: 3827361**		
Note:	Lide (2007) reported various physical-chemical properties and only the confidence of 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	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 13. Refractive Index Summary for Trichloroethylene

Study Reference:	**O'Neil, MJ; Smith, A; Heckelman, PE. (2001). Trichloroethylene. In Merck Index. Whitehouse Station, NJ: Merck & Co., Inc.** **HERO ID: 3809347**		
Note:	O'Neil (2001) reported the refractive index of trichloroethylene.		
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 14. Dielectric Constant Summary for Trichloroethylene

Study Reference:	**Weast, RC; Shelby, SM. (1966). CRC Handbook of Chemistry and Physics Ethene, Trichloro. Cleveland, OH: The Chemical Rubber Co.** **HERO ID: 3809382**		
Note:	Weast and Shelby (1966) reported the dielectric constant of trichloroethylene.		
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**