



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>1,1,2-Trichloroethane</b>
<b>CAS #:</b>	<b>79-00-5</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	August 31, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	133.4	133.41	EPI	EXP
<b>Physical State at ambient temp</b>	Liquid	Liquid	MDEQ	
<b>Melting Point (°C)</b>	238	-36.60	EPI	EXP
<b>Boiling Point (°C)</b>	113.8	113.80	EPI	EXP
<b>Solubility (ug/L)</b>	4.42E+6	4590000	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	25.08	2.30E+01	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	9.13E-4	8.24E-04	EPI	EXP
<b>Log Kow (log P; octanol-water)</b>	2.05	1.89	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	50.3	60.7	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.078	6.69E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.8E-6	1.00E-05	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
Flash Point (°C)	NA	32	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.06	0.06	CRC	EXP
Critical Temperature (K)		6.02E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		8.32E+03	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		1.4397	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.47E-05	2.65E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	5.22E-05	5.92E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	3.46E-05	4.16E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	7.04E-05	9.00E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	3.9E-3	4.0E-4	PPRTV, 2011/MDEQ, 2015	
RfD details	<p>Mouse subchronic drinking water study. NOAEL = 3.9 mg/kg (20 ppm); LOAEL = 44 mg/kg (200 ppm); Critical effects = changes in serum clinical chemistry. UF = 1,000; (White et al., 1985; Sanders et al., 1985).</p>	<p><b>Tier 2 Source:</b>  <b>PPRTV:</b>  <b>Basis:</b> PPRTV is a chronic value and a more current assessment than IRIS. PPRTV subchronic p-RfD = 4.0E-3 mg/kg-day. MDEQ applied an additional UF of 10 was applied to account for use of a subchronic study. Per PPRTV, the IRIS RfD of 4.0E-3 did not consider UF for database deficiencies (UFD) as this RfD was derived before application of a UFD became standard practice.  <b>Critical Studies:</b>                      1) White, K.L., Jr., V.M. Sanders, V.W. Barnes, G.M. Shopp, Jr. and A.E. Munson. 1985. Toxicology of 1,1,2-trichloroethane in the mouse. Drug Chem. Toxicol. 8(5): 333-355.                      2) Sanders, V.M., K.L. White, Jr., G.M. Shopp, Jr. and A.E. Munson. 1985. Humoral and cell-mediated immune status of mice exposed to 1,1,2- trichloroethane. Drug Chem. Toxicol. 8(5): 357-372.  <b>Methods:</b> CD-1 mice (16/sex/group) were exposed to 0, 20, 200, or 2000 mg/L 1,1,2-trichloroethane in drinking water for 90 days (0, 4.4, 46, and 305 mg/kg-day for males and 0, 3.9, 44, and 384 mg/kg-day for females (White et al., 1985; Sanders et al., 1985). Groups of 24 mice of each sex served as controls.  <b>Critical effect:</b> hepatotoxicity (significant increases in serum cholesterol in high-dose males and females, ALP in high-dose males, and ALT and liver weight [without evidence of enzyme induction] in high-dose females.  <b>End point or Point of Departure (POD):</b> NOAEL = 3.9 mg/kg-day  <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and database deficiencies)  <b>Source and date:</b> PPRTV, 4/01/2011</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (2/1/1995), RfD = 4.0E-3 mg/kg-day. The derivation is shown below. Note that the UF value did not include a UF for database deficiencies.  <b>Critical Studies:</b></p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>1) Sanders, V.M., K.L. White, Jr., G.M. Shopp, Jr. and A.E. Munson. 1985. Humoral and cell-mediated immune status of mice exposed to 1,1,2- trichloroethane. Drug Chem. Toxicol. 8(5): 357-372.</p> <p>2) White, K.L., Jr., V.M. Sanders, V.W. Barnes, G.M. Shopp, Jr. and A.E. Munson. 1985. Toxicology of 1,1,2-trichloroethane in the mouse. Drug Chem. Toxicol. 8(5): 333-355.</p> <p><b>Methods:</b> Mice of both sexes were exposed to 1,1,2-TCA in drinking water for 90 days. Concentrations provided were 0, 20, 200, or 2000 mg/L, which resulted in intakes of 0, 4.4, 46, and 305 mg/kg/day for males and 0, 3.9, 44, and 384 mg/kg/day for females.</p> <p><b>Critical effect:</b> changes in clinical serum chemistry indicative of hepatotoxicity in female mice</p> <p><b>End point or Point of Departure (POD):</b> NOAEL = 3.9 mg/kg-day (20 mg/L in females)</p> <p><b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study)</p> <p><b>MRL:</b> Per ATSDR List (April 2015) no chronic oral MRL value at this time. An acute oral MRL is available aRfD = 0.3 mg/kg/day. An Intermediate MRL = 4.0E-2 mg/kg-day for hepatic effects and UF = 100 was derived on 12/1989.</p> <p><b>Critical Study:</b> White KL Jr, Sanders VM, Barnes DW, et al. 1985. Toxicology of 1,1,2-trichloroethane in the mouse. Drug Chem Toxicol 8:333-356.</p> <p><b>Methods:</b> 90-day drinking water study with mice was performed in which the doses consumed were 4.4, 46, and 305 mg/kg for males and 3.9, 44, and 384 mg/kg for females</p> <p><b>Critical effect:</b> liver effects</p> <p><b>End Point or Point of Departure (POD):</b> NOAEL 4.4 mg/kg.day</p> <p><b>Uncertainty Factors:</b> UF = 100; 10 for each intra- and interspecies extrapolation</p> <p><b>Source and date:</b> ATSDR 12/1989</p> <p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b> Per DEQ-CCD (5/26/1988), RRD adopted IRIS RfD. See Part 201 Value details.</p> <p><b>MDEQ:</b> Per DEQ-CCD/WRD (8/27/2012) RfD = 0.0039 mg/kg/day. NOAEL of 0.02 mg/ml (3.9 mg/kg/d) in female CD-1 mice exposed via the drinking water for 90 days</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		(UF=1000) (White et al. 1985).		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	2.9E-2	5.7E-2	IRIS, 1994	
<b>CSF details</b>	Hepatocellular carcinomas in male B6C3F1 mice following treatment by gavage for 5 days/week for 78 weeks (NCI, 1978). Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. CCD/RRD date: 1/18/2000.	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is a Tier 1 value.                      IRIS CSF = 5.7E-2 (mg/kg-day)<sup>-1</sup>. The derivation is shown below.  <b>Critical Study:</b> NCI (National Cancer Institute). 1978. Bioassay of 1,1,2-trichloroethane for possible carcinogenicity. U.S. DHEW Tech. Rep. Ser. 74. Publ. No. NCI-CG-TR- 74.  <b>Methods:</b> Osborne-Mendel rats and B6C3F1 mice were exposed to 1,1,2-trichloroethane by gavage in corn oil: 50/species/sex/dose for each of 2 doses and 20 animals/species/sex for each of 2 control groups. Administration was 5 times/week for 78 weeks during which time doses for rats were increased from 70 and 30 mg/kg/day to 100 and 50 mg/kg/day and doses for mice were increased from 300 and 150 mg/kg/day to 400 and 200 mg/kg/day.</p> <p>1) <i>Dose response data: Tumor Type</i> - hepatocellular carcinoma; <i>Test Species</i> - Mouse/B6C3F1; <i>Route</i> - gavage</p> <p>2) <i>Extrapolation method:</i> Linearized multistage procedure, extra risk</p> <p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> C (Possible Human Carcinogen)  <b>IRIS WOE Basis:</b> based on statistically significant increases in hepatocellular carcinoma in B6C3F1 mice and pheochromocytomas in female B6C3F1 mice (NCI, 1978)  <b>Source and Date:</b> IRIS, 2/01/1994</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> PPRTV (4/01/2011) refers to the IRIS CSF.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/WRD CSF = 0.029 (mg/kg/day)<sup>-1</sup>. Hepatocellular carcinomas in male B6C3F1 mice following treatment by gavage for 5 days/week for 78 weeks (NCI,</p>	Complete	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		1978).		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ( $\mu\text{g}/\text{m}^3$ )	--	2.0E-4	PPRTV, 2011	
RfC/ITSL details	NA	<p><b>Tier 3 Source:</b>  <b>PPRTV Screening Value:</b>  <b>Basis:</b> PPRTV is the only available value. The screening toxicity value in an appendix to a PPRTV assessment is considerably more uncertainty compared with a PPRTV provisional p-RfC.                      PPRTV screening chronic RfC = <math>2.0\text{E}-4 \mu\text{g}/\text{m}^3</math> is derived as follows.  <b>Critical Study:</b> WIL Research Laboratories. (2002). A 90-day inhalation study of 1,1,2-trichloroethane (1,1,2-TCE) in rats (with satellite groups for pharmacokinetic evaluations in rats and mice). Final Report. WIL-417002 (unpublished)  <b>Methods:</b> Groups of 8-week-old Fischer 344 CDF (F344) CrI:BR rats (10/sex/group) were exposed by whole-body inhalation to 0 (filtered air), 15, 40, or 100 ppm of 1,1,2-trichloroethane (99.55% pure) vapor (measured concentrations) 6 hours/day, 5 days/week, for 13 weeks (minimum of 65 exposures). Duration-adjusted concentrations were 0, 14.6, 39.0, and 97.5 mg/m<sup>3</sup> (e.g., 15 ppm <math>\times</math> 5.46 mg/m<sup>3</sup> per ppm <math>\times</math> 6/24 hour's <math>\times</math> 5/7 days = 14.6 mg/m<sup>3</sup>).  <b>Critical effect:</b> vacuolation/micro cysts in male rats  <b>End point or Point of Departure (POD):</b> NOAEL = 15 ppm; NOAEL<sub>ADJ</sub> = 14.6 mg/m<sup>3</sup>; BMDL<sub>10ADJ</sub> = 3.9 mg/m<sup>3</sup>; BMDL<sub>HEC</sub> = 0.51 mg/m<sup>3</sup>  <b>Uncertainty Factors:</b> UF = 3,000 (10 each for intraspecies variability, use of a subchronic study, and database deficiencies and 3 for interspecies extrapolation)  <b>Source and date:</b> PPRTV, 4/1/2011</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (12/01/1992), no value at this time.  <b>MRL:</b> Per ATSDR List (April 2015), no inhalation MRL at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time.		
<b>Inhalation Unit Risk Factor (IURF) ((<math>\mu\text{g}/\text{m}^3</math>)<sup>-1</sup>)</b>	1.6E-5	1.6E-5	IRIS, 1994	
<b>IURF details</b>	IRSL based on hepatocellular carcinomas in mice reported by NCI 1978, calc'd by USEPA in IRIS. CCD/AQD date: 10/15/1992	<p><b>Tier 1 Source:</b> <b>IRIS:</b> <b>Basis:</b> IRIS is the only value available and a Tier 1 source. <b>IRIS IURF = 1.6E-5 (<math>\mu\text{g}/\text{m}^3</math>)<sup>-1</sup></b> is based on the oral exposure data NCI (1978) in the oral exposure cancer risk section of the IRIS file. See Updated Value CSF details. <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> C (Possible Human Carcinogen) <b>IRIS WOE Basis:</b> based on statistically significant increases in hepatocellular carcinoma in B6C3F1 mice and pheochromocytomas in female B6C3F1 mice (NCI, 1978) <b>Source and Date:</b> IRIS, 2/01/1994</p> <p><b>Tier 2 Sources:</b> <b>PPRTV:</b> PPRTV (4/1/2011) refers to the IRIS IURF value. Per PPRTV, a PBPK model for 1,1,2-trichloroethane in rats and mice was developed (The Sapphire Group, 2003) based on previous work (Gargas and Andersen, 1989) and new Pharmacokinetic studies (Poet et al., 2003). The model, applied for extrapolation of the NCI (1978) cancer data from oral-to-inhalation exposure, predicted that the 195-mg/kg-day (5 days/week) cancer LOAEL in the NCI (1978) study was equivalent to a continuous inhalation exposure concentration of 27 ppm. <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, AQD adopted IRIS value for IURF.</p>	Complete	
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	NO	USEPA, 2015	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes/ Issues
<b>MMOA Details</b>	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	No, the RfD and RFC/ITSL are not based on a reproductive-developmental effect.	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<b>State Drinking Water Standard (SDWS) (ug/L)</b>	5	5	SDWA, 1976	
<b>SDWS details</b>	SDWA, 1976	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (ug/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	SDWA, 1976; USEPA SMCL List		
<b>Is there an aesthetic value for drinking water? (Y/N)</b>	NO	Not evaluated	NA	
<b>Aesthetic value (ug/L)</b>	NA	NA	NA	
<b>Aesthetic Value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated	NA	
<b>Phytotoxicity details</b>	NA	NA	NA	
<b>Others</b>				

**(C) Chemical-specific Absorption Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes/ Issues
Gastrointestinal absorption efficiency value (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS <sub>gi</sub> details		RAGS E (EPA, 2004) Default Value		
Skin absorption efficiency value (AE <sub>d</sub> )	---	0.1	MDEQ, 2015	
AE <sub>d</sub> details				
Ingestion Absorption Efficiency (AE <sub>i</sub> )		1.0	MDEQ, 2015	
AE <sub>i</sub> Details				
Relative Source Contribution for Water (RSC <sub>w</sub> )		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC <sub>s</sub> )		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC <sub>A</sub> )		1.0	MDEQ, 2015	
Others				

**(D) Rule 57 Water Quality Values and GSI Criteria**

<b>Current GSI value (µg/L)</b>	330 (X)
<b>Updated GSI value (µg/L)</b>	330 (X)
<b>Rule 57 Drinking Water Value (µg/L)</b>	12

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	110	9/2012
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	3,000	9/2012
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	12	9/2012
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	330	9/2012
<b>Final Chronic Value (FCV)</b>	730	9/2012
<b>Aquatic maximum value (AMV)</b>	3,200	9/2012
<b>Final Acute Value (FAV)</b>	6,400	9/2012

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)



**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	50	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	1	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	3.00E-01	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	9.80E+00	MDEQ, 2015

**CHEMICAL UPDATE WORKSHEET ABBREVIATIONS:**

CAS # - Chemical Abstract Service Number.

**Section (A) Chemical-Physical Properties****Reference Source(s):**

CRC	Chemical Rubber Company Handbook of Chemistry and Physics, 95th edition, 2014-2015
EMSOFT	USEPA Exposure Model for Soil-Organic Fate and Transport (EMSOFT) (EPA, 2002)
EPA2001	USEPA (2001) Fact Sheet, Correcting the Henry's Law Constant for Soil Temperature. Office of Solid Waste and Emergency Response, Washington, D.C.
EPA4	USEPA (2004) User's Guide for Evaluating Subsurface Vapor Intrusion into Buildings. February 22, 2004.
EPI	USEPA's Estimation Programs Interface SUITE 4.1, Copyright 2000-2012
HSDB	Hazardous Substances Data Bank
MDEQ	Michigan Department of Environmental Quality
NPG	National Institute for Occupational Safety and Health Pocket Guide to Chemical Hazards
PC	National Center for Biotechnology Information's PubChem database
PP	Syracuse Research Corporation's PhysProp database
SCDM	USEPA's Superfund Chemical Data Matrix
SSG	USEPA's Soil Screening Guidance: Technical Background Document, Second Edition, 1996
USEPA/EPA	United States environmental protection agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

W9 USEPA's User Guide for Water9 Software, Version 2.0.0, 2001

**Basis/Comments:**

EST	estimated
EXP	experimental
EXT	extrapolated
NA	not available or not applicable
NR	not relevant

**Section (B) Toxicity Values/Benchmarks****Sources/References:**

ATSDR	Agency for Toxic Substances and Disease Registry
CALEPA	California Environmental Protection Agency
CAL DTSC	California Department of Toxic Substances Control
CAL OEHHA	CAEPA Office of Environmental Health Hazard Assessment
CCD	MDEQ Chemical Criteria Database
ECHA	European Chemicals Agency (REACH)
OECD HPV	Organization for Economic Cooperation and Development HPV Database
HEAST	USEPA's Health Effects Assessment Summary Tables
IRIS	USEPA's Integrated Risk Information System
MADEP	Massachusetts Department of Environmental Protection
MDEQ/DEQ	Michigan Department of Environmental Quality
DEQ-CCD/AQD	MDEQ Air Quality Division
DEQ-CCD/RRD	MDEQ Remediation and Redevelopment Division
DEQ-CCD/WRD	MDEQ Water Resources Division
MNDOH	Minnesota Department of Health
NJDEP	New Jersey Department of Environmental Protection

NYDEC	New York State Department of Environmental Conservation
OPP/OPPT	USEPA's Office of Pesticide Programs
PPRTV	USEPA's Provisional Peer Reviewed Toxicity Values
RIVM	The Netherlands National Institute of Public Health and the Environment
TCEQ	Texas Commission on Environmental Quality
USEPA	United States Environmental Protection Agency
USEPA OSWER	USEPA Office of Solid Waste and Emergency Response
USEPA MCL	USEPA Maximum Contaminant Level
WHO	World Health Organization
WHO IPCS	International Programme on Chemical Safety (IPCS/INCHEM)
WHO IARC	International Agency for Research on Cancers
NA	Not Available.
NR	Not Relevant.

**Toxicity terms:**

BMC	Benchmark concentration
BMCL	Lower bound confidence limit on the BMC
BMD	benchmark dose
BMDL	Lower bound confidence limit on the BMD
CSF	Cancer slope Factor
CNS	Central nervous system
IURF or IUR	Inhalation unit risk factor
LOAEL	Lowest observed adverse effect level
LOEL	Lowest observed effect level
MRL	Minimal risk level (ATSDR)
NOAEL	No observed adverse effect level
NOEL	No observed effect level
RfC	Reference concentration

RfD	Reference dose
p-RfD	Provisional RfD
aRfD	Acute RfD
UF	Uncertainty factor
WOE	Weight of evidence

**Section (C) Chemical-specific Absorption Factors**

MDEQ	Michigan Department of Environmental Quality
USEPA RAGS-E	United States Environmental Protection Agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

**Section (D) Rule 57 Water Quality Values and GSI Criteria**

GSI	Groundwater-surface water interface
NA	A value is not available or not applicable.
ID	Insufficient data to derive value
NLS	No literature search has been conducted