CHEMICAL UPDATE WORKSHEET

Chemical Name:	**1,1,1,2-Tetrachloroethane**
CAS #:	**630-20-6**
Revised By:	RRD Toxicology Unit
Revision Date:	August 19, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	167.85	167.85	Epi	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	203	-70.20	EPI	EXP
Boiling Point (˚C)	130.5	130.20	EPI	EXP
Solubility (ug/L)	1.10E+6	1070000	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	12.16	1.20E+01	EPI	EXP
HLC (atm-m³/mol at 25˚C)	2.40E-3	2.50E-03	EPI	EXP
Log Kow (log P; octanol-water)	2.63	2.93	PP	EST
Koc (organic carbon; L/Kg)	145	86.03	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.071	4.82E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	7.9E-6	9.10E-06	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
Flash Point (˚C)	NA	NA	NA	NA
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		6.24E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		9.77E+03	EPA2004	EXP
Density (g/mL, g/cm^3)		1.5406	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	2.30E-05	2.69E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	4.30E-05	6.17E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	3.17E-05	4.24E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	5.57E-05	9.48E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	8.9E-2	3.0E-2	IRIS, 1996	
RfD details	Rat chronic gavage study. LOAEL = 125 mg/kg (adjusted for gavage schedule) = 89.3 mg/kg. Critical effects = mineralization of kidneys in males, hepatic cell change in females. UF = 3000, 3-fold for lack of adequate supporting data. (NTP, 1983). NOTE: it appears that a UF of 1,000 was used. CCD/RRD date: 4/16/1987	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is a chronic value and a Tier 1 source.. **Critical Study**: NTP (National Toxicology Program). 1983. Carcinogenesis studies of 1,1,1,2- tetrachloroethane in F344/N rats and B6C3F1 mice. NTP, Washington, DC. **Methods**: F344/N rats (50/sex/group) were exposed by gavage to 0, 125, or 250 mg/kg/day of technical grade 1,1,1,2- tetrachloroethane in corn oil 5 days/week for 103 weeks. B6C3F1 mice (50/sex/group) were exposed by gavage to 0, 250, or 500 mg/kg/day of technical 1,1,1,2- tetrachloroethane in corn oil 5 days/week for 103 weeks (control and low-dose mice) or 65 weeks (high-dose mice). **Critical effect**: Mineralization of the kidneys in males and hepatic clear cell change in females **End point or Point of Departure (POD):** LOAEL = 125 mg/kg/day converted to 89.3 mg/kg/day **Uncertainty Factors**: UF = 3,000 (10 each for intraspecies variability, interspecies extrapolation, and use of a LOAEL, and 3 for database inadequacies). **Source and date:** IRIS, Last revision date: 12/1/1996. An USEPA review in 2006 did not identify any significant new studies**.** **Tier 2 Sources:** **PPRTV:** PPRTV (9/30/2009) refers to the IRIS RfD. A subchronic RfD = 9.0E-2 mg/kg-day is derived as follows: **Critical Study:** NTP (National Toxicology Program). 1983. Carcinogenesis studies of 1,1,1,2- tetrachloroethane in F344/N rats and B6C3F1 mice. NTP, Washington, DC. **Method(s):** F344/N rats (50/sex/group) were exposed by gavage to 0, 125, or 250 mg/kg/day of 1,1,1,2- tetrachloroethane in corn oil, 5 days/week for 103 weeks. B6C3F1 mice (50/sex/group) were exposed by gavage to 0, 250, or 500 mg/kg/day of 1,1,1,2- tetrachloroethane in corn oil, 5 days/week for		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		103 weeks (control and low-dose mice) or 65 weeks (high-dose mice). **Critical effect:** Reduced survival in males and clinical signs of neurotoxicity End point or Point of Departure (POD): NOAEL = 125 mg/kg-day in rats; $NOAEL_{ADJ}$ = 89.3 mg/kg-day **Uncertainty Factors:** UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation, and database inadequacies). **Source and date:** PPRTV, 9/30/2009. The RfD is calculated from a LOAEL of 125 mg/kg-day (adjusted to 89.3 mg/kg-day) for liver and kidney lesions. Per PPRTV, the kidney lesions were considered to be related to hyaline droplet nephropathy as determined by NTP (1996). Thus, for this PPRTV, USEPA has followed the recommendations of NTP and considers the nephropathy in male rats to not be relevant to humans. **MRL:** No MRL record is available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/RRD (4/16/1987), RfD = 8.9E-2 mg/kg-day. See Part 201 Value RfD details.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	1.1E-2	2.6E-2	IRIS, 1991	
CSF details	Class C. Mouse gavage study (NTP, 1983). Hepatocellular adenomas/carcinomas in females. SF adjusted with revised species scaling factor (70/0.32) rose to the 0.25 power. CCD/RRD date: 3/9/2000.	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only value and a Tier 1 source. **Critical Study**: NTP (National Toxicology Program). 1983. Carcinogenesis studies of 1,1,1,2- tetrachloroethane in F344/N rats and B6C3F1 mice. NTP, Washington, DC. **Method(s)**: See Updated Value RfD details. 1) *Dose response data*: *Tumor Type* - hepatocellular adenoma or carcinoma; *Test Species* - mouse/B6C3F1, female; *Route* - gavage 2) *Extrapolation method*: Linearized multistage procedure, extra risk **Carcinogen Weight-of-Evidence (WOE) Class**: C; possible human carcinogen **IRIS WOE Basis**: increased incidence of combined hepatocellular adenomas and carcinomas in female mice; inadequate evidence from human studies **Source and Date**: IRIS, Last revision date – 1/01/1991		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Tier 2 Sources: **PPRTV:** PPRTV (9/30/2009) refers to the IRIS value. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/RRD (3/9/2000), CSF = 1.1E-2 $(mg/kg\text{-}day)^{-1}$. See Part 201 Value CSF details.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu g/m^3$)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	**Tier 1 and 2 Sources:** **IRIS:** Per IRIS (12/01/1996), no value at this time. **PPRTV:** Per PPRTV (9/30/2009), no value at this time. **MRL:** No MRL record is available at this time. **Tier 3 Sources:** **MDEQ:** Per DEQ-CCD, no value at this time.		Complete
Inhalation Unit Risk Factor (IURF) ($(\mu g/m^3)^{-1}$)	7.4E-6	7.4E-6	IRIS, 1991	
IURF details	Potency in IRIS is based on NTP 1983 gavage study with male mice had increased incidences of hepatocellular carcinomas and	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is a Tier 1 source. IRIS IUR was derived by extrapolation of the oral data presented in Updated Value CSF details. **Carcinogen Weight-of-Evidence (WOE) Class**: C; possible human carcinogen **IRIS WOE Basis**: increased incidence of combined hepatocellular adenomas and carcinomas in female mice; inadequate evidence from human studies **Source and Date**: IRIS, Last revision date – 1/01/1991		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	adenomas. CCD-AQD date: 5/4/1988.	**Tier 2 Sources:** **PPRTV:** PPRTV (9/30/2009) refers to the IRIS value. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/AQD (5/4/1988), IURF = 7.4E-6 $(\mu g/m^3)^{-1}$ See Part 201 Value IURF details.		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	No. The RfD and RfC/ITSL are not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (ug/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399.		
Secondary Maximum Contaminant Level (SMCL) (ug/L)	--	NO	SDWA, 1976 and USEPA SMCL List, 2015	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015.		
Is there an aesthetic value for drinking water? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value (ug/L)	NA	NA	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Aesthetic Value details	NA	NA		
Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	NA	NA	
Others				

(C) Chemical-specific Absorption Factors

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABSgi)	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABSgi details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (AEd)	---	0.1	MDEQ, 2015	
AEd details				
Ingestion Absorption Efficiency (AEi)		1.0	MDEQ, 2015	
AEi Details				
Relative Source Contribution for Water (RSC_W)		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC_S)		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC_A)		1.0	MDEQ, 2015	
Others				

(D) Rule 57 Water Quality Values and GSI Criteria

Current GSI value (µg/L)	ID
Updated GSI value (µg/L)	ID
Rule 57 Drinking Water Value (µg/L)	19

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	680	03/2002
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	3,500	03/2002
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	19	03/2002
Human Cancer values for non-drinking water source (HCV-Non-drink)	100	03/2002
Final Chronic Value (FCV)	ID	03/2002
Aquatic maximum value (AMV)	ID	03/2002
Final Acute Value (FAV)	ID	03/2002

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 website
2. MDEQ Rule 57 table

(E) Target Detection Limits (TDL)

	Value	Source
Target Detection Limit – Soil (μg/kg)	100	MDEQ, 2015
Target Detection Limit – Water (μg/L)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	5.10E-01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	1.70E+01	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