



CHEMICAL UPDATE WORKSHEET

Chemical Name:	1,1,1-Trichloroethane
CAS #:	71-55-6
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)	133.4	133.41	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	241	-30.41	EPI	EXP
Boiling Point (°C)	74	74.00	EPI	EXP
Solubility (ug/L)	1.33E+6	1290000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	121.6	1.24E+02	EPI	EXP
HLC (atm-m³/mol at 25°C)	1.72E-2	1.72E-02	EPI	EXP
Log Kow (log P; octanol-water)	2.48	2.49	EPI	EXP
Koc (organic carbon; L/Kg)	110	43.89	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.078	6.48E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.8E-6	9.60E-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)	0.075	0.08	CRC	EXP
Critical Temperature (K)		545.00	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		7.14E+03	EPA2001	EXP
Density (g/mL, g/cm³)		1.339	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm²)	2.65E-05	2.80E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm²)	6.28E-05	6.81E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm²)	3.76E-05	4.45E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm²)	8.82E-05	1.08E-04	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	2.2E+0	2.0E+0	IRIS, 2007	
RfD details	<p>Fischer rats and B6C3F1 mice were exposed to 0, 150, 500, or 1,500 ppm via inhalation for 6 hr/day, 5 days/week for 2 yrs. Female rats in the 1500 ppm grp. exhibited decreased b.w. and both male and females exhibited very slight microscopic changes in the liver. No adverse effects were noted in mice at any dose level. The NOAELs for rats and mice were 500 and 1500 pm, resp. 500 ppm = 216 mg/kg/d (absorption factor of 45% and inhalation rate of</p>	<p>Tier 1 Source: IRIS: Basis: IRIS is Tier 1 source. IRIS RfD = 2.0E+0 mg/kg/day. Critical Study: NTP. (2000) NTP technical report on the toxicity studies of 1,1,1-trichloroethane (CAS no.71 55 6) administered in microcapsules in feed to F344/N rats and B6C3F1 mice. Public Health Service, U.S. Department of Health and Human Services; NTP Toxicity Report Series No. 41. Available from the National Institute of Environmental Health Sciences, Research Triangle Park, NC, and the National Technical Information Service, Springfield, VA; PB2001 100476. Methods: Groups of 10 male and 10 female F344/N rats and B6C3F1 mice were fed diets containing 0 (untreated feed), 0 (placebo microcapsules), 5000, 10,000, 20,000, 40,000, or 80,000 ppm of microencapsulated 1,1,1-trichloroethane 7 days/week for 13 weeks. Average daily doses were 290, 600, 1200, 2400, and 4800 mg/kg in male rats; 310, 650, 1250, 2500, and 5000 mg/kg in female rats; 850, 1770, 3500, 7370, and 15,000 mg/kg in male mice; and 1340, 2820, 5600, 11,125, and 23,000 mg/kg in female mice. Critical effect: reduced terminal body weight End point or Point of Departure (POD): BMDL₁₀ = 2,155 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability and interspecies extrapolation and 3 each for use of a subchronic study and database deficiency) Source and date: IRIS, Last revision date - 9/28/2007. An IRIS Toxicological Review is available. Tier 1 and 2 Sources: PPRTV: No PPRTV record is available at this time. MRL: Per ATSDR List (April 2015), no chronic MRL at this time. An Intermediate MRL = 2.0E+1 mg/kg-day was derived using the NTP (2000) study:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	0.931 m ³ /kg/d). UF of 100 used. CCD/RRD date: 5/19/1997	<p>Critical Study: NTP, 2000. Technical report on the toxicity studies of 1,1,1-trichloroethane (CAS No. 7155-6) administered in microcapsules in feed to F344/N rats and B6C3F1 mice. National Toxicology Program. (41) NIH 004402.</p> <p>Methods: Groups of male and female B6C3F1 mice (10 per group) were fed diets containing 0 (untreated feed); 0 (microcapsule vehicle in feed); 5,000; 10,000; 20,000; 40,000; or 80,000 ppm of microencapsulated 1,1,1-trichloroethane (99% pure) 7 days/week for 13 weeks. Average daily doses were 850; 1,750; 3,500; 7,370; and 15,000 mg/kg in male mice; and 1,340; 2,820; 5,600; 11,125; and 23,000 mg/kg in female mice. Clinical signs and body weights were recorded weekly.</p> <p>Critical effect: decreased terminal body weight in female mice</p> <p>End point or Point of Departure (POD): BMDL10 = 2,185 mg/kg-day</p> <p>Uncertainty Factors: UF = 100 (10 each for intraspecies variability and interspecies extrapolation)</p> <p>Source and date: ATSDR, final 7/2006</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/RRD, RfD = 2.2E+0 mg/kg-day. See Part 201 Value RfD details.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: "inadequate information to assess carcinogenic potential."</p> <p>IRIS WOE Basis: Epidemiologic studies of humans chronically exposed to 1,1,1-trichloroethane are inconclusive. A 2-year inhalation bioassay showed no treatment-related increase in tumors in rats and mice at an exposure concentration below the maximum tolerated dose. The two available oral cancer bioassays in rats and mice are considered inadequate for evaluation of carcinogenic potential.</p> <p>Source and Date: IRIS, 9/28/2007</p> <p>Tier 1 and 2 Sources:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>IRIS: Per IRIS (9/28/2007), no value at this time. PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD, no value at this time.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	1.0E+3	5.0E+3	IRIS, 2007	
RfC/ITSL details	The EPA (96-007d/8-09-96) developed a provisional RfC of $1000 \mu\text{g}/\text{m}^3$ based on a 3-month continuous inhalation exposure in gerbils (Rosengren et al., 1985).	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 value. 1,1,1-Trichloroethane IRIS, 2007, RfC= $5.0\text{E}+3 \mu\text{g}/\text{m}^3$. Critical Studies: 1) Quast, JF; Calhoun, LL; McKenna, MJ. (1984) Chlorothene VG: a chronic inhalation toxicity and oncogenicity study in rats and mice (part 1 and 2) with cover letter dated 082184. The Dow Chemical Company, Midland, MI. Submitted under TSCA Section 4; EPA Document No. 40-8424496; NTIS No. OTS0510656. 2) Quast, JF; Calhoun, LL; Frauson, LE. (1988) 1,1,1-Trichloroethane formulation: a chronic inhalation toxicity and oncogenicity study in Fischer 344 rats and B6C3F1 mice. Fundam Appl Toxicol 11:611—625. 3) McNutt, NS; Amster, RL; McConnell, EE; et al. (1975) Hepatic lesions in mice after continuous inhalation exposure to 1,1,1-trichloroethane. Lab Invest 32:642—654. Methods: 1) Quast et al. (1988, 1984) exposed groups of 80 male and 80 female F344 rats and B6C3F1 mice to 0, 150, 500, or 1500 ppm (0, 820, 2730, or 8190 mg/m^3) production-grade (94%) 1,1,1-trichloroethane vapor for 6 hours/day, 5 days/week for 2 years. Ten rats and 10 mice of each sex from each exposure group were scheduled for interim sacrifices after 6, 12, and 18 months of exposure, and the remaining 50 rats and 50 mice/sex/group were scheduled for</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>sacrifice after 24 months of exposure.</p> <p>2) McNutt et al. (1975) chamber-exposed male CF-1 mice to 0, 250, or 1000 ppm (0, 1370, or 5460 mg/m³) technical grade 1,1,1-trichloroethane (94—97% pure, 2.4—3.0% dioxane, 0.12—0.30% butanol) continuously for up to 14 Serial sacrifices were performed on 10 mice/concentration at weekly intervals during the exposure period and at post exposure weeks 2 and 4.</p> <p>Critical effect: Liver histopathologic changes</p> <p>End point or Point of Departure (POD): NOAEL_{HEC} = 1,553</p> <p>Uncertainty Factors: UF = 100 (10 each for intraspecies variability and interspecies extrapolation)</p> <p>Note: Because the chronic RfC based on liver histopathologic changes following repeated exposure (16 mg/m³) was higher than the short-term RfC (5 mg/m³), the chronic RfC was set at 5 mg/m³ so as not to exceed the limiting reference value derived for short-term exposure. The short-term RfC applies to exposures for more than 24 hrs. up to 30 days.</p> <p>Source and date: IRIS, Last revision date - 9/28/2007. An IRIS Toxicological Review is available.</p> <p>Tier 2 Sources:</p> <p>PPRTV: No PPRTV record is available at this time.</p> <p>MRL: Per ATSDR List (April 2015), no chronic MRL value is available at this time. An Intermediate MRL = 0.7 ppm was derived as follows:</p> <p>Critical Study: Rosengren LE, Aurell A, Kjellstrand P, et al. 1985. Astrogliosis in the cerebral cortex of gerbils after long-term exposure to 1,1,1-trichloroethane. Scand J Work Environ Health 11:447-456.</p> <p>Methods: Groups of Mongolian gerbils (four/sex) were exposed to 70, 210, or 1,000 ppm of 1,1,1-trichloroethane vapor (cleaning grade, containing 5% dioxane-free stabilizers) continuously for 3 months. Each exposure group was paired with a control group consisting of eight sex-matched littermates of the test group. At the end of the exposure period, all animals were held for 4 months prior to sacrifice.</p> <p>Critical effect: biochemical changes (increased GFA protein) in the brain indicative</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>of neuronal damage. End point or Point of Departure (POD): NOAEL_{HEC} = 70 ppm Uncertainty Factors: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) Source and date: ATSDR, final 7/2006</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD/AQD RfC = 6000 µg/m³. Per AQD (9/28/2007): The EPA (2007) developed new RfC with 24-hour averaging based on MacKay et al (1987) and PBPK modeling of humans exposed with neurobehavioral changes. There also was 1, 4, and 8 hour RfC's developed. Because AQD usually assigns 24 hour averaging times to RfC's, the 24-hour RfC was used as the ITSL.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m³)⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: "inadequate information to assess carcinogenic potential." IRIS WOE Basis: Epidemiologic studies of humans chronically exposed to 1,1,1-trichloroethane are inconclusive. A 2-year inhalation bioassay showed no treatment-related increase in tumors in rats and mice at an exposure concentration below the maximum tolerated dose. The two available oral cancer bioassays in rats and mice are considered inadequate for evaluation of carcinogenic potential. Source and Date: IRIS, 9/28/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (9/28/2007), no value at this time. PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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 or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (ug/L)	200	200	SDWA, 1976	
SDWS details	SDWA, 1976	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		
Is there an aesthetic value for drinking water? (Y/N)	NO	Not evaluated	NA	
Aesthetic value (ug/L)	NA	NA	NA	
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 (ABS_{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS_{gi} details		RAGS E (EPA, 2004) Default Value		
Skin absorption efficiency value (AE_d)	---	0.1	MDEQ, 2015	
AE_d details				
Ingestion Absorption Efficiency (AE_i)		1.0	MDEQ, 2015	
AE_i 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)	89
Updated GSI value (µg/L)	89
Rule 57 Drinking Water Value (µg/L)	62,000

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	62,000	8/2012
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	1,300,000	8/2012
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	NA
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	NA
Final Chronic Value (FCV)	89	7/2012
Aquatic maximum value (AMV)	800	7/2012
Final Acute Value (FAV)	1,600	7/2012

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 ($\mu\text{g}/\text{kg}$)	50	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.10E+03	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	3.60E+04	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 OEHHHA	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

