



CHEMICAL UPDATE WORKSHEET

Chemical Name:	1,1,2-Trichloro-1,2,2-trifluoroethane
CAS #:	76-13-1
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	187.38	187.38	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	237	-35.00	EPI	EXP
Boiling Point (°C)	47.7	47.70	EPI	EXP
Solubility (ug/L)	1.70E+5	170000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	364.8	3.63E+02	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	5.30E-1	3.16E-01	CRC	EXP
Log Kow (log P; octanol-water)	3.15	3.16	EPI	EXP
Koc (organic carbon; L/Kg)	1250	196.8	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.078	3.76E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.2E-6	8.59E-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)		487.30	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		6.46E+03	EPA2004	EXP
Density (g/mL, g/cm ³)		1.5635	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	2.68E-05	2.80E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	6.49E-05	6.84E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	3.82E-05	4.46E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	9.17E-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)	2.7E+1	2.7E+1	IRIS, 1996	
RfD details	NOTE: copy CCD The RfD (2.7E+1 mg/kg/d) differs from the IRIS reported RfD (3E+1 mg/kg/d) in that two significant figures are presented. CCD/RRD date: /1985	<p>Tier 1 Source: IRIS: Basis: The IRIS RfD was selected because it represents the most recent assessment. Critical Study: Imbus, H.R. and C. Adkins. 1972. Physical examination of workers exposed to trichlorotrifluoroethane. Arch. Environ. Health. 24(4): 257-261. Methods: A group of 50 workers, exposed for an average of 2.77 years in an environment, samples of which contained from 46 to 4,700 ppm of trichlorotrifluoroethane (Freon 113), was examined. Critical effect: psychomotor impairment End point or Point of Departure (POD): NOAEL = 273 mg/kg/day (converted from 5358 mg/m³; 5358 mg/m³ x 10 m³/day x 5 days/7 days x 0.5 absorption factor/70 kg BW) Uncertainty Factors: UF = 10 for intraspecies variability Source and date: IRIS, Last revision date - 2/01/1996. An IRIS screening level review in 2002 did not identify any critical new studies.</p> <p>Tier 2 Sources: PPRTV: No PPRTV record is available at this time. MRL: No MRL record is available at this time.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD, RRD adopted IRIS RfD. See Part 201 Value RfD details. Per CCD/WRD (7/2000), RfD = .1E+1 mg/kg-day based on the Imus and Adkins (1972) study and UF = 10 MDEQ: Per DEQ-CCD/WRD (7/6/2000), RfD = 21 mg/kg/day. A NOAEL of 699 ppm (208 mg/kg/d) in humans exposed occupationally for 6 hours/day, 5 days/week, for 2.77 years was reported. An absorption factor of 0.5 and volume of air breathed per 6 hours of 7.5 m³ were used. In addition, an uncertainty factor of</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		10 was used for interhuman variability. (Imbus and Adkins, 1972).		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Tier 1 Source: IRIS: Per IRIS (2/01/1996), no value at this time. IRIS has not evaluated the carcinogenic potential at this time.</p> <p>Tier 2 Sources: PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	7.67E+4	1.9E+4	MDEQ, 2006	
RfC/ITSL details	Complete info	<p>Tier 3 Source: MDEQ: Basis: All other Tier 3 values are based on HEAST and the same study. MDEQ-AQD dosimetrically adjusted the NOAEL to an ambient human equivalent concentration which represents the most up-to-date manipulation of the data. The ITSL was based on a human occupational inhalation study conducted by Imbus and Adkins (1972). The mean exposure concentration of 699 ppm was used to derive an RfC using the 1994 USEPA guidelines. Averaging time = 24 hour. See below for more details.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (2/01/1996), no value at this time. PPRTV: No PPRTV record is available at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>MRL: No MRL record is available at this time.</p> <p>Tier 3 Sources: MDEQ-AQD, 2006: Critical Study: Imbus, H.R. and C. Adkins. 1972. Physical examination of workers exposed to trichlorotrifluoroethane. Arch. Environ. Health. 24(4): 257-261. Method(s): human occupational exposure for 2.77 years Critical effect: psychomotor impairment End point or Point of Departure (POD): NOAEL_{HEC} = 1914 mg/m³ (original NOAEL = 699 ppm). Uncertainty Factors: UF = 100: 10 each for intraspecies variation and extrapolation from sub-chronic to chronic. Source and date: MDEQ-CCD/AQD, 3/23/2006.</p> <p>HEAST: RfC= 3E+1 mg/m³ based on HEAST Summary 1997. Based on Inbus and Atkins (1972).</p> <p>California DTSC: RfC= 3.0E+04 µg/m³ based on HEAST.</p> <p>Minnesota: RfC= 3.00E+01 mg/m³ based on HEAST.</p> <p>Texas CEQ: RfC= 3.0E+01mg/m³ based on HEAST.</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: NTP ROC, health and environmental agencies of Massachusetts, New Jersey and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (2/01/1996), no value at this time. IRIS has not evaluated the carcinogenic potential at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only. Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.		
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)	--	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		
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		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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 (USEPA, 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)	32
Updated GSI value (µg/L)	32
Rule 57 Drinking Water Value (µg/L)	444,000

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	444,000	7/2000
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	1,834,000	7/2000
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)	32	6/2012
Aquatic maximum value (AMV)	280	6/2012
Final Acute Value (FAV)	570	6/2012

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 ($\mu\text{g}/\text{kg}$)	250	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	2.50E+03	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	8.40E+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