



CHEMICAL UPDATE WORKSHEET

Chemical Name:	2,4,5-Trichlorophenol
CAS #:	95-95-4
Revised By:	RRD Toxicology Unit
Revision Date:	September 9, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	197.5	197.45	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	340	69.00	EPI	EXP
Boiling Point (°C)	247	247.00	EPI	EXP
Solubility (ug/L)	1.20E+6	1200000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.01596	7.50E-03	PC	EXP
HLC (atm-m ³ /mol at 25°C)	4.33E-6	4.33E-06	SSG	EXP
Log Kow (log P; octanol-water)	3.9	3.72	EPI	EXP
Koc (organic carbon; L/Kg)	1597	1777	EPI	EST
Ionizing Koc (L/kg)		2365	SSG	EST
Diffusivity in Air (Di; cm ² /s)	0.0291	3.31E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	7.03E-6	8.69E-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	133	PC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		759.13	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		1.10E+04	EPA2001	EST
Density (g/mL, g/cm ³)		1.678	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm²)	3.56E-07	1.43E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm²)	3.56E-07	1.43E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm²)	4.24E-07	1.81E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm²)	4.24E-07	1.81E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.0E-1	3.0E-2	PPRTV, 2007	
RfD details	Rat oral chronic in feed study. Not clear if 10% conversion factor is study specific.....assume d so. NOAEL = 100 mg/kg; LOAEL = 300 mg/kg; Critical effect = liver & kidney pathology. UF = 1000 (McCollister et al., 1961). CCD/RRD date:	<p>Tier 2 Source: PPRTV: Basis: PPRTV provisional subchronic RfD is based on a more recent assessment. MDEQ applied an additional UF of 10 for subchronic to chronic extrapolation to derive the chronic RfD. See below. PPRTV, 7/27/2007: Critical Study: McCollister, D.D., D.T. Lockwood and J.K. Rowe. 1961. Toxicological information on 2,4,5-trichlorophenol. Toxicol. Appl. Pharmacol. 3:63-70. Method(s): Wistar rats (10/sex/group) were exposed to diets containing 0, 0.01, 0.03, 0.1, 0.3 or 1% 2,4,5-trichlorophenol for 98 days. Daily dose estimates were calculated to be 0, 10, 30, 100, 300 and 1000 mg/kg-day. Critical effect: degenerative histopathological changes in the liver (cloudy swelling and focal necrosis) and kidney (degeneration of tubule epithelium) and a diurnal effect observed in male and female rats. End point or Point of Departure (POD): NOAEL = 100 mg/kg-day Uncertainty Factors: UF = 300 (10 each for intraspecies variability and interspecies extrapolation, and 3 for database deficiencies)</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (3/1/1988), RfD = 1.0E-1 derived as follows: Critical Study: McCollister, D.D., D.T. Lockwood and J.K. Rowe. 1961. Toxicological information on 2,4,5-trichlorophenol. Toxicol. Appl. Pharmacol. 3:63-70. Method(s): Wistar rats (10/sex/group) were exposed to diets containing 0, 0.01, 0.03, 0.1, 0.3 or 1% (levels from 100 through 10,000 ppm) 2,4,5-trichlorophenol for 98 days. Critical effect: liver and kidney pathology. End point or Point of Departure (POD): NOAEL = 100 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation, and use of a subchronic study).</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Source and date: IRIS, Last revision date - 3/1/1988. A September 2001 USEPA screening level review did not identify any critical new studies.</p> <p>MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/RRD (5/20/1985), RfD = 1.0E-1 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 evidence to assess the carcinogenic potential</p> <p>IRIS WOE Basis: Human studies have not evaluated cancer risks of exposure to 2,4,5-trichlorophenol as a single agent. No conclusion could be derived from the available genotoxicity studies. No other studies were available that evaluated the carcinogenic potential of 2,4,5-trichlorophenol.</p> <p>Source and Date: PPRTV, 7/27/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (3/1/1998), no value at this time. PPRTV: Per PPRTV (7/27/2007), no value 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/m ³)	3.5E+2	3.5E+2	MDEQ, 1996	
RfC/ITSL details	Groups of 10/sex Wistar rats	<p>Tier 3 Source: MDEQ:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	<p>received 2,4,5-tcp in the diet for 98 days, resulting in a NOAEL of 100 mg/kg/d per R232(1)(b) [UF=1000] (McCollister, 1961). CCD/AQD date: 3/25/1996.</p>	<p>Basis: MDEQ was the only value returned in the Tier 3 search. Based on the McCollister, et al. (1961) oral study. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (7/1/1991), no value at this time. Information reviewed but value not estimated. PPRTV: Per PPRTV (7/27/2007), no value at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ-AQD, 1996: Critical Study: McCollister, D.D., D.T. Lockwood and J.K. Rowe. 1961. Toxicological information on 2,4,5-trichlorophenol. Toxicol. Appl. Pharmacol. 3:63-70. Method(s): Wistar rats (10/sex/group) were exposed to diets containing 0, 0.01, 0.03, 0.1, 0.3 or 1% 2,4,5-trichlorophenol for 98 days. Daily dose estimates were calculated to be 0, 10, 30, 100, 300 and 1000 mg/kg-day. Critical effect: degenerative histopathological changes in the liver (cloudy swelling and focal necrosis) and kidney (degeneration of tubule epithelium) and a diurnal effect observed in male and female rats. End point or Point of Departure (POD): NOAEL = 100 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study) Source and date: MDEQ-CCD/AQD, 3/25/1996</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: inadequate evidence to assess the carcinogenic potential</p> <p>IRIS WOE Basis: Human studies have not evaluated cancer risks of exposure to 2,4,5-trichlorophenol as a single agent. No conclusion could be derived from the available genotoxicity studies. No other studies were available that evaluated the carcinogenic potential of 2,4,5-trichlorophenol.</p> <p>Source and Date: PPRTV, 7/27/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (3/1/1998), no value at this time. PPRTV: Per PPRTV (7/27/2007), no value 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
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	--	NO	SDWA, 1976 and USEPA SMCL List	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(SMCL) (ug/L)				
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		
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	
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)	NA
Updated GSI value (µg/L)	NA
Rule 57 Drinking Water Value (µg/L)	NA

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

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 ($\mu\text{g}/\text{kg}$)	330	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	5	MDEQ, 2015
Target Detection Limit – Air (ppbv)	NA	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	NA	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