



CHEMICAL UPDATE WORKSHEET

Chemical Name:	2,4,6-Trichlorophenol (DD)
CAS #:	88-06-2
Revised By:	RRD Toxicology Unit
Revision Date:	August 31, 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)	342	69.00	EPI	EXP
Boiling Point (°C)	246	246.00	EPI	EXP
Solubility (ug/L)	8.00E+5	800000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.0114	8.00E-03	PC	EXP
HLC (atm-m³/mol at 25°C)	7.79E-6	7.79E-06	SSG	EXP
Log Kow (log P; octanol-water)	3.7	3.69	EPI	EXP
Koc (organic carbon; L/Kg)	381	1777	EPI	EST
Ionizing Koc (L/kg)		1040	SSG	EST
Diffusivity in Air (Di; cm²/s)	0.0318	3.31E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	6.25E-6	8.68E-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	99	PC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		749.03	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		1.20E+04	EPA2001	EST
Density (g/mL, g/cm ³)		1.675	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	6.26E-07	1.92E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	6.26E-07	1.92E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	7.46E-07	2.43E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	7.46E-07	2.43E-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-02	PPRTV, 2007/MDEQ, 2016	
RfD details	NA	<p>Tier 2 Source: PPRTV: Basis: No Tier 1 available. PPRTV (3/21/2007) RfD = 1.0E-03 mg/kg-day. Removed the 10-fold UF for use of a subchronic study since the effect is developmental and single event pregnant female and child will be used as receptors. Critical Study: Exon, J.H. and L.D. Koller. 1985. Toxicity of 2-chlorophenol, 2,4-dichlorophenol, and 2,4,6-trichlorophenol. In: Water Chlorination: Chemistry, Environmental Impact and Health Effects, R.L. Jolley et al., Ed. Proceedings Fifth Conference Williamsburg, Chelsea, MI. Lewis Publishers. p. 307-330. Methods: reproductive toxicity study - female Sprague-Dawley rats were exposed to 2,4,6-TCP in drinking water for 10 weeks prior to mating (weanlings when started) and continuing throughout mating and gestation. Critical effect: decreased litter size End point or Point of Departure (POD): NOAEL = 3.0 mg/kg-day Uncertainty Factors: UF = 3,000 (10 each for intraspecies variability, interspecies extrapolation, and 3 for database deficiencies). MDEQ removed the 10-fold UF for use of a subchronic study. Source and date: PPRTV, 3/21/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (7/1/1991), no value at this time. MRL: No MRL record is available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/WRD, RfD = 0.08 mg/kg/day. Critical study: Bercz, J.P., M. Robinson, L. Jones et al. 1990. Subchronic toxicity studies of 2,4,6-trichlorophenol in Sprague-Dawley rats. J. Am. Coll. Toxicol. 9(5): 497-506. Methods: In a subchronic gavage study, groups of 10 male and 10 female</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Sprague-Dawley rats, 49 days of age, were administered 2,4,6-TCP in oral doses of 0, 80, 240, or 720 mg/kg-day by gavage (in corn oil) for 90 days.</p> <p>Critical effect: increased absolute or relative liver weight in mid- and high-dose males and females and increased absolute and relative kidney weight in high-dose males</p> <p>End point or Point of Departure (POD): NOAEL = 80 mg/kg-day</p> <p>Uncertainty factors: UF =1000; 10 each for intra- and intraspecies variability and use of subchronic study</p> <p>Source and Date: DEQ-CCD/WRD 12/8/2006</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	7.4E-3	1.1E-02	IRIS, 1994	
CSF details	<p>Increase in leukemia in male rats exposed via the diet. Liver tumor data in mice could not be used because dioxins were present in the diet and they may have caused the tumors (NCI, 1979). Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. RRD calculation date: 1/18/2000.</p>	<p>Tier 1 Source:</p> <p>IRIS:</p> <p>Basis: IRIS is a Tier 1 source.</p> <p>IRIS CSF = 1.1E-02 (mg/kg-day)⁻¹.</p> <p>Critical Study: NCI (National Cancer Institute). 1979. Bioassay of 2,4,6-Trichlorophenol for Possible Carcinogenicity. U.S. DHEW Publ. No. NCI-CG-TR-155.</p> <p>Methods: 2,4,6-TCP was added to the diet of 50 each male and female F344 rats and B6C3F1 mice (NCI, 1979). Rats were exposed to 5000 or 10,000 ppm 2,4,6-TCP in feed for 106 or 107 weeks. Male mice received 5000 or 10,000 ppm of 2,4,6- TCP for 105 weeks. Female mice were initially administered 10,000 or 20,000 ppm of 2,4,6- TCP in feed. As the animals were observed to have decreased body weights, these concentrations were lowered to 2500 and 5000 ppm at week 38 (TWA dose = 5214 or 10,428 ppm).</p> <p>1) <i>Dose response data:</i> Tumor Type - leukemia; Test Species - rat/F344, male; Route - diet</p> <p>2) <i>Extrapolation method:</i> Linearized multistage procedure, extra risk</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen</p> <p>IRIS WOE Basis: Based on no human data and sufficient evidence in animals; namely, increased incidence of lymphomas or leukemias in male rats and hepatocellular adenomas or carcinomas in male and female mice</p> <p>Source and Date: IRIS, Last revision date – 2/01/1994</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Tier 2 Sources: PPRTV: Per PPRTV (3/21/2007), no value at this time. Refers to IRIS value. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD/RRD (1/18/2000), CSF = 7.4E-3 (mg/kg-day)⁻¹. See Part 201 Value CSF details.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (2/1/1994), no value at this time. PPRTV: Per PPRTV (3/21/2007), no value at this time. MRL: No MRL record is available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Inhalation Unit Risk Factor (IURF) ((µg/m³) ⁻¹)	3.1E-6	3.1E-6	IRIS, 1994	
IURF details	Based on the incidence of leukemia in male rats following treatment via the diet (NCI, 1979), as listed in IRIS. CCD/AQD, 11/05/1992.	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS IURF = 3.1E-6 (µg/m³)⁻¹. This value was derived from the oral data. Critical Study: NCI (National Cancer Institute). 1979. Bioassay of 2,4,6-Trichlorophenol for Possible Carcinogenicity. U.S. DHEW Publ. No. NCI-CG-TR-155. Methods: 2,4,6-TCP was added to the diet of 50 each male and female F344 rats and B6C3F1 mice (NCI, 1979). Rats were exposed to 5000 or 10,000 ppm 2,4,6-TCP in feed for 106 or 107 weeks. Male mice received 5000 or 10,000 ppm of 2,4,6-TCP for 105 weeks. Female mice were initially administered 10,000 or</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>20,000 ppm of 2,4,6- TCP in feed. As the animals were observed to have decreased body weights, these concentrations were lowered to 2500 and 5000 ppm at week 38 (TWA dose = 5214 or 10,428 ppm).</p> <p>3) <i>Dose response data: Tumor Type - leukemia; Test Species - rat/F344, male; Route - diet</i></p> <p>4) <i>Extrapolation method: Linearized multistage procedure, extra risk</i></p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen IRIS WOE Basis: Based on no human data and sufficient evidence in animals; namely, increased incidence of lymphomas or leukemias in male rats and hepatocellular adenomas or carcinomas in male and female mice Source and Date: IRIS, Last revision date – 2/01/1994</p> <p>Tier 2 Sources: PPRTV: Per PPRTV (3/21/2007), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, AQD adopted the IRIS value. See Part 201 Value IURF details.</p>		
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	YES-oral, the RfD is based on a reproductive-developmental effect. Oral Exposure Pathways- Single Exposure.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	<p>Critical effect: decreased litter size Critical Study: Exon, J.H. and L.D. Koller. 1985. Toxicity of 2-chlorophenol, 2,4-dichlorophenol, and 2,4,6-trichlorophenol. In: Water Chlorination: Chemistry, Environmental Impact and Health Effects, R.L. Jolley et al., Ed. Proceedings Fifth Conference Williamsburg, Chelsea, MI. Lewis Publishers. p. 307-330. Methods: female Sprague-Dawley rats were exposed to 2,4,6-TCP in drinking</p>		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		water for 10 weeks prior to mating (weanlings when started) and continuing throughout mating and gestation.		
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 SMCL List	
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	
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)	5
Updated GSI value (µg/L)	5
Rule 57 Drinking Water Value (µg/L)	41

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	1,900	12/2006
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	14,000	12/2006
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	41	12/2006
Human Cancer values for non-drinking water source (HCV-Non-drink)	290	12/2006
Final Chronic Value (FCV)	5	9/2006
Aquatic maximum value (AMV)	39	9/2006
Final Acute Value (FAV)	79	9/2006

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 ($\mu\text{g}/\text{L}$)	4	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 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