



CHEMICAL UPDATE WORKSHEET

Chemical Name:	4,4'-DDT(DD)
CAS #:	50-29-3
Revised By:	RRD Toxicology Unit
Revision Date:	August 17, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	354.49	354.49	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	382	108.50	EPI	EXP
Boiling Point (°C)	260	260.00	EPI	EXP
Solubility (ug/L)	25	5.5	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.0000003952	1.60E-07	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	8.10E-6	8.32E-06	EPI	EXP
Log Kow (log P; octanol-water)	6.53	6.91	EPI	EXP
Koc (organic carbon; L/Kg)	1.78E+5	1.686E+05	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.0137	2.29E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	4.95E-6	5.8531E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	162 F	72.2	NPG	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		720.75	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		2.20E+04	EPA2001	EST
Density (g/mL, g/cm ³)		1.56	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	1.07E-08	1.60E-07	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	1.07E-08	1.60E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	1.19E-08	1.99E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	1.19E-08	1.99E-07	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	5.0E-4	5.0E-4	ATSDR, 2008	
RfD details	<p>27-week rat feeding study (Laug et al., 1950); NOAEL = 0.05 mg/kg/day based on conversion of 1ppm dose by 5% bw/day food consumption rate UF=100. Critical effect = liver lesions. Source: IRIS. CCD date: 2/18/1985.</p>	<p>Tier 2 Source: ATSDR: Basis: ATSDR (9/2002, addendum 11/2008) oral acute MRL and oral intermediate MRL = 5.0E-4 mg/kg-day. The acute MRL is mainly considered because the acute exposure study generated a more sensitive effect: neurodevelopment toxicity. The IRIS (1996) RfD value is similar to the ATSDR value and used the same critical study. 1) MRL: Per ATSDR (2002), an oral acute MRL = 5.0E-4 is based on results from a group of studies conducted by the same group of investigators in which the most significant finding was the presence of altered motor behavior in adult mice treated with DDT perinatally: Critical Studies: Eriksson and Nordberg 1986; Eriksson et al. 1990a, 1990b, 1992, 1993; Johansson et al. 1995, 1996; Talts et al. 1998. Methods: Groups of 10-day-old male NMRI mice were treated by gavage with a single dose of 0 (vehicle control) or 0.5 mg DDT/kg in a fat emulsion vehicle by gavage (Eriksson et al. 1990a). At the age of 4 months, the mice were subjected to behavioral tests of spontaneous activity (locomotion, rearing, and total activity). Tests were conducted for 1 hour, and scores were summed for three 20-minute periods. Previous studies have shown a significant increase in density of MACH in the cerebral cortex of 10-day-old mice 7 days after dosing, but not at 1 day post-exposure compared to controls (Eriksson and Nordberg 1986). In a follow-up study, Eriksson et al. (1992) treated 3-, 10-, and 19-day-old mice, and conducted behavioral testing and neurochemical evaluations at 4 months of age. Critical effect: neurodevelopmental effects (increase in spontaneous motor activity). Perinatal exposure decreased the density of muscarinic cholinergic receptors in the cerebral cortex and increased spontaneous motor activity in adults. End point or Point of Departure (POD): LOAEL = 0.5 mg/kg. Uncertainty Factors: UF = 1000 (10 each for interspecies variability, interspecies</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>extrapolation and use of a LOAEL) Source and date: ATSDR 2002 Toxicological Profile for DDT, DDD and DDE and 11/2008 Addendum for DDT/DDD/DDE (supplement to the Tox Profile)</p> <p>2) MRL: Per ATSDR (9/2002), oral intermediate MRL = 5.0E-4 mg/kg-day. Critical Study: Laug, E.P., A.A. Nelson, O.G. Fitzhugh and F.M. Kunze. 1950. Liver cell alteration and DDT storage in the fat of the rat induced by dietary levels of 1-50 ppm DDT. J. Pharmacol. Exp. Therap. 98: 268-273; Fitzhugh O, Nelson A. 1947. The chronic oral toxicity of DDT (2,2-bis(p-chlorophenyl)1,1,1-trichloroethane). J Pharmacol Exp Ther 89:18-30. Methods: Osborne-Mendel rats (15/sex/group) were exposed to 0, 1, 5, 10, or 50 ppm technical DDT (dissolved in corn oil) added to the diet for 15–27 weeks. This study was essentially designed to examine whether DDT accumulates in adipose tissue and to what extent, how age and dose level affect accumulation, and how rapidly it is eliminated. Seventy-seven rats were used for microscopic evaluation of only the liver and kidney. This was based on findings from a previous study from the same group (Fitzhugh and Nelson 1947, see below) in which higher dietary levels of DDT had been used. Based on the previous findings, only the liver was expected to show microscopic changes. Critical effect: Liver effects (lesions) End point or Point of Departure (POD): NOAEL = 1 ppm in food = 1 mg/kg = 0.05 mg/kg/day. Uncertainty Factors: UF = 100 (10 each for interspecies variability and interspecies extrapolation) Source and date: ATSDR 2002 Toxicological Profile for DDT, DDD and DDE and 11/2008 Addendum for DDT/DDD/DDE (supplement to the Tox Profile)</p> <p>Tier 1 and 2 Sources: IRIS: IRIS (2/1/1996) RfD = 5.0E-4 mg/kg-day. Critical Study: Laug, E.P., A.A. Nelson, O.G. Fitzhugh and F.M. Kunze. 1950. Liver cell alteration and DDT storage in the fat of the rat induced by dietary levels of 1-50 ppm DDT. J. Pharmacol. Exp. Therap. 98: 268-273.</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Method: Weanling rats (25/sex/group) were fed 1, 5, 10 or 50 ppm commercial DDT in corn oil solution with powdered chow for 15- 27 weeks</p> <p>Critical effect: liver lesions (increased hepatocellular hypertrophy, increased cytoplasmic oxyphilia, and peripheral basophilic cytoplasmic granules)</p> <p>End point or Point of Departure (POD): NOAEL = 1 ppm (0.05 mg/kg bw/day)</p> <p>Uncertainty Factors: UF = 100 (10 each for interspecies variability and interspecies extrapolation)</p> <p>Source and date: IRIS, Last revision date - 2/1/1996. A USEPA screening-level review in 2002 identified one or more significant new studies.</p> <p>PPRTV: No PPRTV record available at this time.</p> <p>MRL: Per ATSDR (9/2002), oral MRL for chronic-duration exposure to DDT was not derived because of the inadequacy of the available data on liver effects in animals to describe the dose-response relationship at low-dose levels. In a brief communication, Fitzhugh (1948) stated that histopathological lesions occurred in the liver of rats fed 10 ppm DDT in the diet for 2 years, but no experimental details were given, so the quality of the study cannot be evaluated. Using reference values for body weight and food consumption from EPA (1988), the 10 ppm dietary level was approximately 0.7 mg/kg/day. This dietary level was still higher than the lowest level resulting in hepatic effects in the Laug et al. 1950 study used for derivation of the intermediate-duration MRL.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, RRD adopted IRIS value (3/20/1985).</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	2.0E-1	3.4E-1	IRIS, 1991	
CSF details	Several mouse & rat chronic studies (See IRIS). Quantitative estimate is	<p>Tier 1 Source: Basis: IRIS is a Tier 1 source. Critical Studies: Turusov et al., 1973; Terracini et al., 1973; Thorpe and Walker, 1973; Tomatis and Turusov, 1975; Cabral et al., 1982; Rossi et al., 1977 Methods: Ten slope factors derived from six studies were within a 13-fold range.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	geometric mean of 10 slope factors. Benign & malignant liver tumors in mice and rats. Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. Source: IRIS. CCD date: 3/20/2000.	<p>The slope factor derived from the mouse data alone was 4.8E-1 while that derived from the rat data alone was 1.5E-1. A geometric mean of the slope factors from the mouse and rat data was used for the overall slope factor of 3.4E-1, which was identical for the same tumor site as that for DDE [3.4E-1 per (mg/kg)/day], a structural analog.</p> <p>1) <i>Dose response data: Tumor Type</i> – benign and malignant liver tumors; <i>Test Species</i> – mouse and rat; <i>Route</i> - oral (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 IRIS WOE Basis: Observation of tumors (generally of the liver) in seven studies in various mouse strains and three studies in rats. DDT is structurally similar to other probable carcinogens, such as DDD and DDE. Source and Date: IRIS, Last revision date - 5/1/1991. A USEPA screening-level review in 2002 identified significant new studies.</p> <p>Tier 2 Sources: PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD/RRD (3/20/2000), CSF = 2.0E-1 (mg/kg-day)⁻¹, a modified IRIS value. See Part 201 Value CSF details. MDEQ: Per DEQ-CCD/WRD (3/1/1995), CSF = 3.40E-1 (mg/kg-day)⁻¹ based on EPA CSF.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	Tier 1 and 2 Sources: IRIS: Per IRIS (2/01/1996), no value at this time.		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>PPRTV: No PPRTV record available at this time. MRL: Per ATSDR (09/2002), no inhalation value at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$)⁻¹)	9.7E-5	9.7E-5	IRIS, 1999	
IURF details	Potency in EPA IRIS is the geometric mean of several oral studies that found liver tumors. Oral potency was converted to air value. CCD/AQD date: 6/24/1987	<p>Tier 1 Source: Basis: IRIS is a Tier 1 source. IRIS IURF = $9.7\text{E}-5$ ($\mu\text{g}/\text{m}^3$)⁻¹. The IURF is based on the oral data (see below) Critical Studies: Turusov et al., 1973; Terracini et al., 1973; Thorpe and Walker, 1973; Tomatis and Turusov, 1975; Cabral et al., 1982; Rossi et al., 1977 Method(s): Ten slope factors derived from six studies were within a 13-fold range. The slope factor derived from the mouse data alone was $4.8\text{E}-1$ while that derived from the rat data alone was $1.5\text{E}-1$. A geometric mean of the slope factors from the mouse and rat data was used for the overall slope factor of $3.4\text{E}-1$, which was identical for the same tumor site as that for DDE [$3.4\text{E}-1$ per (mg/kg)/day], a structural analog.</p> <p>3) <i>Dose response data:</i> Tumor Type – benign and malignant liver tumors; <i>Test Species</i> – mouse and rat; <i>Route</i> - oral (diet)</p> <p>4) <i>Extrapolation method:</i> linearized multistage procedure, extra risk</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen IRIS WOE Basis: based on studies showing increased incidence of tumors (generally liver). Source and Date: IRIS, Last revision date - 5/1/1991. A USEPA screening-level review in 2002 identified significant new studies.</p> <p>Tier 2 Sources: PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		MDEQ: Per DEQ-CCD, AQD adopted IRIS value for IURF (6/24/1987).		
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: neurodevelopmental effects (increase in spontaneous motor activity). Perinatal exposure decreased the density of muscarinic cholinergic receptors in the cerebral cortex and increased spontaneous motor activity in adults.</p> <p>Critical Studies: Eriksson and Nordberg 1986; Eriksson et al. 1990a, 1990b, 1992, 1993; Johansson et al. 1995, 1996; Talts et al. 1998.</p> <p>Method(s): Groups of 10-day-old male NMRI mice were treated by gavage with a single dose of 0 (vehicle control) or 0.5 mg DDT/kg in a fat emulsion vehicle by gavage (Eriksson et al. 1990a). At the age of 4 months, the mice were subjected to behavioral tests of spontaneous activity (locomotion, rearing, and total activity). Tests were conducted for 1 hour, and scores were summed for three 20-minute periods. Previous studies have shown a significant increase in density of MACH in the cerebral cortex of 10-dayold mice 7 days after dosing, but not at 1 day post-exposure compared to controls (Eriksson and Nordberg 1986). In a follow-up study, Eriksson et al. (1992) treated 3-, 10-, and 19-day-old mice, and conducted behavioral testing and neurochemical evaluations at 4 months of age.</p>		
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	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)	---	0.03	USEPA RAGS-E	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		0.5	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)	0.02 (M); 0.000011
Updated GSI value (µg/L)	0.02 (M); 0.000011
Rule 57 Drinking Water Value (µg/L)	0.02 (M); 0.00015

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	0.002	7/1997
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	0.002	7/1997
Wildlife Value (WV)	0.000011	7/1997
Human Cancer Values for Drinking Water Source (HCV-drink)	0.00015	7/1997
Human Cancer values for non-drinking water source (HCV-Non-drink)	0.00015	7/1997
Final Chronic Value (FCV)	0.0032	8/1997
Aquatic maximum value (AMV)	0.029	8/1997
Final Acute Value (FAV)	0.057	8/1997

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 ($\mu\text{g}/\text{kg}$)	20	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	0.02	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