



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Propachlor
CAS #:	1918-16-7
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)	211.69	211.69	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	---	77.00	EPI	EXP
Boiling Point (°C)	---	110	PP	EXP
Solubility (ug/L)	6.55E+5	580000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.00023	2.30E-04	EPI	EXP
HLC (atm-m³/mol at 25°C)	1.09E-7	3.60E-07	PP	EST
Log Kow (log P; octanol-water)	2.01	2.18	EPI	EXP
Koc (organic carbon; L/Kg)	94.6	204.50	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.08	2.68E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.0E-6	6.96E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	NA	NA	NA	NA
Lower Explosivity Level (LEL; unitless)	NA	NA	NA	NA
Critical Temperature (K)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm ³)		1.242	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.10E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	1.10E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	1.39E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	1.39E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.3E-2	5.4E-2	OPP, 1998	
RfD details	<p>The RfD is based on a subchronic rat feeding study (Monsanto Co., 1964). Twenty-five rats/sex/dose were fed concentrations of propachlor (as 65% wettable powder) in the diet that were calculated to equal 0, 1.3, 13.3, and 133.3 mg/kg/day. Dietary concentrations were adjusted weekly so as to maintain the desired dosages. CRITICAL EFFECT = The only apparent effects of treatment were decreases in body weights in males and females of</p>	<p>Tier 1 Source: EPA-OPP: Basis: The OPP RfD is selected since it is based on a 2-year study while the IRIS RfD is based on a 90-day study. Critical Study: EPA-OPP; On May 7, 1997, after reviewing chronic studies in rats, mice, and dogs, the RfD for propachlor was determined to be 0.054 mg/kg/day, based on the rat chronic toxicity study [MRID 44168301; full reference not in the two docs save in file] with a NOEL of 5.4 mg/kg/day. (The LOEL was 16.1 mg/kg/day, based on stomach lesions in males and liver lesions in both sexes.) An uncertainty factor of 100 (previously determined appropriate by the HED RfD Committee) was applied to account for both inter-species extrapolation and intraspecies variability. Methods: Two year feed study in rats. Propachlor [97.83% a.i.] was administered to 60 F-344 rats/sex/dose via the diet at dose levels of 0, 100, 300, 1000, and 2500 [males]/5000 [females] ppm [males 0, 5.4, 16.1, 53.6, and 125.3/females 0, 6.4, 19.3, 65.5, and 292.1 mg/kg/day, respectively] for 24 months. Due to palatability problems, the high dose level was attained by ramping the dose from 1000 ppm initially to the desired level by increasing by 500 ppm each week. Critical Effect: based on stomach lesions in males and liver lesions in both sexes End point or Point of Departure (POD): NOEL = 5.4 mg/kg/day; LOEL = 16.1 mg/kg/day). Uncertainty Factors: UF = 100; 10-fold for both inter-species extrapolation and intraspecies variability Source and date: EPA-OPP; 11/1998</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/1/1992), RfD = 1.3E-2 mg/kg-day Critical Study: Monsanto Company. 1964a. MRID No. 00093270; HED Doc. No. 001381. Available from EPA. Write to FOI, EPA, Washington DC 20460</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	10-12%, and increases in relative liver weights of about 10%. NOAEL = 13.3 mg/kg-d. Total UF = 1,000 (10 each for intraspecies variability and interspecies and subchronic to chronic extrapolation). The RfD was last revised: 1/1/92.	<p>(unpublished). Method(s): 90 day feeding study in rats. Twenty-five rats/sex/dose were fed concentrations of propachlor (as 65% wettable powder) in the diet that were calculated to equal 0, 1.3, 13.3, and 133.3 mg/kg/day. Dietary concentrations were adjusted weekly so as to maintain the desired dosages. The effects of treatment on body weight gain, food consumption, hematology, urinalysis, and gross and microscopic pathology were assessed. The only apparent effects of treatment were decreases in body weights in males and females of 10-12%, and increases in relative liver weights of about 10%. Critical effect: Decreased weight gain, food consumption; increased relative liver weights End point or Point of Departure (POD): NOEL = 13.3 mg/kg/day; LEL = 133.3 mg/kg/day. Uncertainty Factors: UF =1000; 10-fold each for inter- and intraspecies differences, and the insufficient duration of the study to fully assess chronic effects Source and date: IRIS; 1/1/1992</p> <p>PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD (RRD calculation date: 7/22/1986), RfD = 0.013 mg/kg/day. NOAEL = 13.3 mg/kg/day; UF = 1000; Critical effects = decreased weight gain, food consumption, increased liver weights. 90-day feeding study in rats, (Monsanto Co., 1964).</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	3.2E-2	OPP, 1998	
CSF details	No RD entry in EPB-CCD (9/16/11). Per IRIS: a	<p>Tier 1 Source: EPA-OPP Basis: OPP is a Tier 1 source. USEPA-OPP CSF = 3.2E-2 (mg/kg-day)⁻¹ based on female rat ovarian tumors.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	quantitative estimate of carcinogenic risk from oral exposure is not available at this time (9/16/11). No PPRTV (11/28/11, 1/10/13).	<p>Critical Studies: MRID 44168301 (not identified in pesticide documents). Methods: In the combined chronic toxicity/carcinogenicity study in rats, propachlor was administered to 60 F0344 rats/sex/dose via the diet at dose levels of 0, 100, 300, 1000, and 25000 (males)/5000 (females) ppm (males 0, 5.4 16.1, 53.6, and 125.3/females 0, 6.4, 19.3, 65.5, and 292.1 mg/kg/day, respectively) for 24 months. The CSF was calculated using a linear low-dose approach, the Tox Risk 4.0 K. Crump model and converting from animals to humans using the ¼'s scaling factor. The largest Q₁* (the Q₁* for male liver tumors also calculated) was estimated to be 3.2E-1. Carcinogen Weight-of-Evidence (WOE) Class: B2 – likely human carcinogen WOE Basis: based on the (1) rare stomach tumor in male Fischer 344 rats; (2) thyroid tumors in male and ovarian granulosa/theca cell tumors in female Sprague-Dawley rats at doses that were not adequate to assess carcinogenicity; (3) hepatocellular tumors in male CD-1 mice; (4) in vitro clastogenic activity; and (5) tumors observed at one or more of the same sites with three structurally-related chloroacetanilide compounds. Source and Date: USEPA-OPP, 11/1998</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (last revision 1/31/1987), no value at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tire 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	NA	MDEQ, 2015	
RfC/ITSL details	No AQD entry in EPB-CCD	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/31/1987), no value at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	(9/16/11). No PPRTV (11/28/11, 1/10/13).	<p>PPRTV: No PPRTV record available at this time. MRL: No MRL record available 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)	--	NA	MDEQ, 2015	
IURF details	No AQD entry in EPB-CCD (9/16/11). No PPRTV (11/28/11, 1/10/13).	<p>Carcinogen Weight-of-Evidence (WOE) Class: B2 – likely human carcinogen WOE Basis: based on the (1) rare stomach tumor in male Fischer 344 rats; (2) thyroid tumors in male and ovarian granulosa/theca cell tumors in female Sprague-Dawley rats at doses that were not adequate to assess carcinogenicity; (3) hepatocellular tumors in male CD-1 mice; (4) in vitro clastogenic activity; and (5) tumors observed at one or more of the same sites with three structurally-related chloroacetanilide compounds. Source: EPA-OPP RED, 11/1998</p> <p>Tier 2 Sources: IRIS: Per IRIS (last revision 1/31/1987), no value at this time. EPA-OPP-RED (11/1998): No value available. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tire 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	No	USEPA, 2014	
MMOA Details	--	Not listed as a carcinogen with a mutagenic mode of action in the USEPA OSWER list.		
Developmental or Reproductive Effector? (Y/N)	NO	No, the RfD is not based on a reproductive-developmental effect; however, there are developmental and reproduction studies reported in the EPA-OPP-RED (11/1998).	MDEQ, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Developmental or Reproductive Toxicity Details	NA	Developmental and reproduction studies are reported in the EPA-OPP-RED (11/1998).		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/L)	--	NO	SDWA, 1976 and USEPA SMCL List	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
Is there an Aesthetic Value? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	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)	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 ($\mu\text{g}/\text{kg}$)	200	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	50	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