



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Simazine
CAS #:	122-34-9
Revised By:	RRD Toxicology Unit
Revision Date:	August 26, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	201.66	201.66	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	---	226.00	EPI	EXP
Boiling Point (°C)	---	NA	NA	
Solubility (ug/L)	4470	6200	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.0000000221	2.21E-08	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	3.37E-9	9.42E-10	PP	EST
Log Kow (log P; octanol-water)	1.93	2.18	EPI	EXP
Koc (organic carbon; L/Kg)	79.0	146.5	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.08	2.81E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.0E-6	7.37E-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)		1.302	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.74E-07	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	1.74E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	1.90E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	1.90E-07	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	5.2E-3	5.0E-3	IRIS, 1994	
RfD details	<p>Chronic (2-year) feeding to rats (Ciba-Geigy Corp., 1988). Critical effect = reduction in weight gain & hematological changes in females. NOAEL=0.52 mg/kg/day; UF=100. CCD/RRD date: 8/14/1991</p>	<p>Basis: The IRIS endpoint was selected because it is based on a chronic study and the systemic, chronic effects are the most sensitive effects.</p> <p>Tier 1 Sources: IRIS, 1994: Critical Study: Ciba-Geigy Corp. 1988a. MRID No. 40614405; HED Doc No. 007240, 007449 Available from EPA. Write to FOI, EPA, Washington, DC 20460.</p> <p>Method(s): Sprague-Dawley rats were fed technical simazine for 2 years at dietary levels of 0, 10, 100 or 1000 ppm (Male: 0, 0.41, 4.2, 45.8 mg/kg-day; Female: 0, 0.52, 5.3, 63.1 mg/kg-day). Animals tested for chronic toxicity effects consisted of 40 rats/sex in the control and high-dose groups and 30/sex in the low- and mid-dose groups, while 50/sex/dose were tested for carcinogenicity. After approximately 52 weeks of treatment in the chronic toxicity test, 10 rats/sex/group were sacrificed and an additional 10 rats/sex from the control and high-dose groups were maintained on an untreated diet for approximately 52 weeks at which time all the remaining animals were sacrificed. After 104 weeks of treatment, all remaining animals from the chronic toxicity and carcinogenicity test were sacrificed.</p> <p>Critical effect: reduction in body weight gain; hematological changes in females End point or Point of Departure (POD): NOAEL = 0.52 mg/kg-day (10 ppm) Uncertainty Factors: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) Source and date: IRIS, Last revision date - 4/01/1994. An EPA screening level review in 2002 identified one or more significant new studies.</p> <p>OPP - Memorandum dated June 4, 2013. Subject: Atrazine, Propazine, and Simazine. Human Health Risk Scoping Document in Support of Registration Review: Acute RfD = 3E-01 mg/kg/day.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Critical Study: Developmental study in rats (MRID 40614403). Infurna, R. (1986) A Teratology Study in Rats: Simazine Technical: Study No. 83058; 822099. Unpublished study prepared by CibaGeigy Corp. 262 p.</p> <p>Methods: Simazine was administered to CR1 female rats by gavage at dose levels of 0, 30, 300, or 600 mg/kg/day from days 6 through 15 of gestation. There were 19 animals in the control and 600 mg/kg groups and 23/dose in the 30 and 300 mg/kg groups.</p> <p>Critical Effects: Increased incidence of unossified teeth, head, centra vertebrae, sternabrae, and also on rudimentary ribs.</p> <p>POD: Developmental NOAEL = 30 mg/kg/day</p> <p>UF: 100</p> <p>Chronic RfD = 1.8E-2 mg/kg/day.</p> <p>Critical Study: MRID No. 44152102 (This MRID was not in the 1/12/2006 RED Memorandum.)</p> <p>Methods: Simazine was administered to 360 female SD rats in the diet. Dose levels were 0, 25, 50, and 400 ppm (0, 1.180, 3.65, 29.44 mg/kg/day) for 26 weeks.</p> <p>Critical Effects: based on estrous cycle alterations and LH surge suppression.</p> <p>POD: NOAEL = 1.8 mg/kg/day. LOAEL = 3.65 mg/kg/day.</p> <p>UF: 100 (10 each for interspecies and intraspecies variability).</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 Source: MDEQ: Per DEQ-CCD (8/14/1991), RRD adopted IRIS RfD. See Part 201 Value RfD details.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day) ⁻¹	--	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
CSF details	NA	<p>Tier 1 Sources: IRIS: Per IRIS (4/1/1994), no value at this time. Carcinogenic potential has not been evaluated.</p> <p>OPP Cancer Assessment Document, April 14, 2005: The committee classified Simazine as “Not Likely to be Carcinogenic to Humans” based on the following: Simazine is not genotoxic and operates via a mode of action for the development of mammary and pituitary tumors in the female SD rat similar to atrazine. Atrazine’s mode of action of tumor formation appears to be specific to female rats (which maintain constant estrus) and does not appear to have a counterpart in humans, and thus the mammary gland and pituitary tumors found in atrazine or simazine treated SD female rats are qualitatively not relevant for human risk assessment.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value 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>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	<p>Tier 1 Source: IRIS: Per IRIS (4/01/1994), no value at this time.</p> <p>OPP Documents (January 2006): Not available at this time.</p> <p>Tier 2 Sources: 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 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	NA	<p>Tier 1 Sources: IRIS: Per IRIS (4/1/1994), no value at this time. Carcinogenic potential has not been evaluated.</p> <p>OPP January 2006 Memorandum: Not available 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
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2014	
MMOA Details	--	<p>NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.</p>		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2014	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (ug/L)	--	4	SDWA, 1976	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
Is there an aesthetic value for drinking water? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value (ug/L)	NO	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, 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)	17
Updated GSI value (µg/L)	17
Rule 57 Drinking Water Value (µg/L)	140

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	140	4/2006
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	4,000	4/2006
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)	17	4/2006
Aquatic maximum value (AMV)	160	4/2006
Final Acute Value (FAV)	310	4/2006

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 ($\mu\text{g}/\text{kg}$)	80	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