



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	alpha-Hexachlorocyclohexane
<b>CAS #:</b>	319-84-6
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	August 18, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	290.82	290.83	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	433	159.50	PP	EXP
Boiling Point (°C)	288	288	PP	EXP
Solubility (ug/L)	2000	2000	PP	EXP
Vapor Pressure (mmHg at 25°C)	0.00004256	3.50E-05	PC	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	1.06E-5	6.70E-06	PP	EXP
Log Kow (log P; octanol-water)	3.8	3.80	PP	EXP
Koc (organic carbon; L/Kg)	1220	2807	EPI	EXT
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.0142	2.75E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	7.34E-6	7.35E-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	65.6	PC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		8.39E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		1.50E+04	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		1.87	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	4.34E-07	1.29E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	4.34E-07	1.29E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	5.17E-07	1.63E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	5.17E-07	1.63E-06	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
<b>Reference Dose (RfD) (mg/kg/day)</b>	--	8.0E-3	ATSDR, 2005	
<b>RfD details</b>		<p><b>Basis:</b> ATSDR chronic oral MRL = 0.008 mg/kg/day. ATSDR is the only value at this time.</p> <p><b>Critical Study:</b> Fitzhugh OG, Nelson AA, Frawley JP. 1950. The chronic toxicities of technical benzene hexachloride and its <math>\alpha</math>, <math>\beta</math> and <math>\gamma</math> isomers. J Pharmacol Exp Ther 100:59-66. (Table 2 of the article).</p> <p><b>Method:</b> Wistar rats (10/sex/group) were treated with 0, 10, 50, 100, or 800 ppm <math>\alpha</math>-HCH in food for life. Estimated doses were 0, 0.7, 3.5, 7, or 56 mg/kg/day in males and 0, 0.8, 4, 8, or 64 mg/kg/day in females.</p> <p><b>Critical Effect:</b> Liver effects</p> <p><b>End point or Point of Departure (POD):</b> NOAEL = 0.8 mg/kg/day (10 ppm)</p> <p><b>Uncertainty Factors:</b> 100; (10 each for interspecies extrapolation and intraspecies variability.</p> <p><b>Source and Date:</b> ATSDR, August 2005. A Toxicological Profile for alpha-, beta-, gamma-, and delta-Hexachlorocyclohexane (HCH) is available.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (07/01/1993), RfD not available at this time.  <b>PPRTV:</b> No PPRTV record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per MDEQ-CCD, no value at this time.</p>		Complete
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	2.0E+0	6.3E+0	IRIS, 1993	
<b>CSF details</b>	Basis: Increased liver tumors in 5 mouse strains & WISTAR rats. SF based on Ito et al., 1973 - hepatic	<p><b>Basis:</b> IRIS is a Tier 1 source.</p> <p><b>Tier 1/IRIS Source:</b>  <b>Critical Study:</b> Ito, N., H. Nagasaki, M. Arai, S. Sugihara and S. Makiura. 1973a. Histologic and ultrastructural studies on the hepatocarcinogenicity of benzene hexachloride in mice. J. Natl. Cancer Inst. 51(3): 817-826.  <b>Method(s):</b> Male dd mice (20-40/group) were treated in the diet with 100, 250,</p>		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
	nodules and carcinomas in male mice. Classification: B2. Recalculated using updated species scaling factor. CCD/RRD date: 7/1/2000	or 500 ppm alpha-HCH for 24 weeks. 1) <i>Dose response data: Tumor Type</i> - hepatic nodules and hepatocellular carcinomas ; <i>Test Species</i> - mouse/dd, male; <i>Route</i> - oral (diet) 2) <i>Extrapolation method</i> : Linearized multistage procedure, extra risk <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> B2; probably human carcinogen. <b>IRIS WOE Basis:</b> increased incidence of liver tumors in five mouse strains and in Wistar rats. <b>Source and Date:</b> IRIS, Last revision date - 07/01/1993.  <b>Tier 2 Sources:</b> <b>PPRTV:</b> No PPRTV record available at this time. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per CCD/RRD (7/1/2000), CSF = 2.0E+0 (mg/kg-day) <sup>-1</sup> . See Part 201 Value CSF details. Per CCC/WRD (1/1/1983), CSF = 4.15E+0 (mg/kg-day) <sup>-1</sup> based on increased liver tumors in male strain dd mice dosed via the diet for 24 weeks (Ito, 1973). Results were corrected for the shortness of study duration.		
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)</b>	NA	NA	MDEQ, 2015	
<b>RfC/ITSL details</b>		<b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (07/01/1993), no value at this time. <b>PPRTV:</b> No PPRTV record available at this time. <b>MRL:</b> Per ATSDR, MRL not available at this time.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD (date), no value at this time.		Complete
<b>Inhalation Unit Risk Factor</b>	1.8E-3	1.8E-3	IRIS, 1993	



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
(IURF) ((µg/m <sup>3</sup> ) <sup>-1</sup> )				
<b>IURF details</b>	IUR based on EPA's IRIS inhalation risk estimate, which is based on the oral data showing liver tumors occurring in 5 mouse strains and Wistar rats following dietary exposure. CCD/AQD date: 7/1/1993	<p><b>Tier 1/IRIS Source:</b>  <b>Basis:</b> Per IRIS, the IURF estimate is based on the Ito et al. (1973) oral data. IRIS is the only available value.  <b>Critical Study:</b> Ito, N., H. Nagasaki, M. Arai, S. Sugihara and S. Makiura. 1973a. Histologic and ultrastructural studies on the hepatocarcinogenicity of benzene hexachloride in mice. J. Natl. Cancer Inst. 51(3): 817-826.  <b>Method(s):</b> Male dd mice (20-40/group) were treated in the diet with 100, 250, or 500 ppm alpha-HCH for 24 weeks.                      3) <i>Dose response data: Tumor Type</i> - hepatic nodules and hepatocellular carcinomas ; <i>Test Species</i> - mouse/dd, male; <i>Route</i> - oral (diet)                      4) <i>Extrapolation method:</i> Linearized multistage procedure, extra risk  <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> B2; probably human carcinogen.  <b>IRIS WOE Basis:</b> increased incidence of liver tumors in five mouse strains and in Wistar rats.  <b>Source and Date:</b> IRIS, Last revision date - 07/01/1993.</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD, (7/1/1993), AQD adopted the IRIS IURF.</p>		Complete
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	No	USEPA, 2014	
<b>MMOA Details</b>	--			
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2014	
<b>Developmental or Reproductive</b>	NA	NA		



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
<b>Toxicity Details</b>				
<b>State Drinking Water Standard (SDWS) (µg/L)</b>	NA	NO	SDWA, 1976	
<b>SDWS details</b>		MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (µg/L)</b>	NA	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>		MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
<b>Is there an aesthetic value for drinking water? (Y/N)</b>	No	Not evaluated.	NA	
<b>Aesthetic value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	No	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA		
<b>Others:</b>				

**(C) Chemical-specific Absorption Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS <sub>gi</sub> details		RAGS E (EPA, 2004) Default Value		
Skin absorption efficiency value (AE <sub>d</sub> )	---	0.1	MDEQ, 2015	
AE <sub>d</sub> details				
Ingestion Absorption Efficiency (AE <sub>i</sub> )		1.0	MDEQ, 2015	
AE <sub>i</sub> Details				
Relative Source Contribution for Water (RSC <sub>w</sub> )		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC <sub>s</sub> )		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC <sub>A</sub> )		1.0	MDEQ, 2015	
Others				

**(D) Rule 57 Water Quality Values and GSI Criteria**

<b>Current GSI value (µg/L)</b>	ID
<b>Updated GSI value (µg/L)</b>	ID
<b>Rule 57 Drinking Water Value (µg/L)</b>	0.05 (M); 0.016

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	19	10/2009
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	21	10/2009
<b>Wildlife Value (WV)</b>	ID* (0.016)	10/2009
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	0.016	10/2009
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	0.017	10/2009
<b>Final Chronic Value (FCV)</b>	ID	10/2009
<b>Aquatic maximum value (AMV)</b>	ID	10/2009
<b>Final Acute Value (FAV)</b>	ID	10/2009

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)

**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	10	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	0.05	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	1.18E-03	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	3.95E-02	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