



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Pentachlorobenzene
CAS #:	608-93-5
Revised By:	RRD Toxicology Unit
Revision Date:	September 21, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	250.3	250.34	EPI	EXP
Physical State at ambient temp	Liquid	Solid	MDEQ	
Melting Point (°C)	357	86.00	EPI	EXP
Boiling Point (°C)	277	277.00	EPI	EXP
Solubility (ug/L)	650	831	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.001672	2.00E-03	PC	EXP
HLC (atm-m³/mol at 25°C)	8.40E-4	7.03E-04	EPI	EXP
Log Kow (log P; octanol-water)	5.26	5.17	EPI	EXP
Koc (organic carbon; L/Kg)	1.48E+5	3708	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.067	2.94E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	6.3E-6	7.95E-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)		1.51E+04	HSDB	EXP
Density (g/mL, g/cm ³)		1.8342	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.16E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	1.19E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	1.50E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	1.51E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	8.3E-4	8.0E-4	IRIS, 1988	
RfD details	<p>Subchronic rat oral bioassay. LOAEL = 8.3 mg/kg; Critical effect = liver and kidney toxicity. 100-fold UF for use of subchronic study and LOAEL; UF = 10,000, (Linder et al., 1980). CCD/RRD date: 10/9/85.</p>	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS RfD = 8.0E-4 mg/kg-day Critical Study: Linder, R., T. Scotti, J. Goldstein, K. McElroy and D. Walsh. 1980. Acute and subchronic toxicity of pentachlorobenzene. J. Environ. Pathol. Toxicol. 4: 183-196. Methods: 8 groups (3 males, 5 females) of 10 rats each were exposed to 0, 125, 1000 ppm (male rats)/ 0,125, 250, 500, 1000 ppm (weanling females) in diet for 100 days (males)/180 days (weanling females). Critical effect: liver and kidney toxicity End point or Point of Departure (POD): LOAEL = 8.3 mg/kg/day Uncertainty Factors: UF = 10,000; (10 each for intra-species variability, interspecies extrapolation, use of a subchronic study and use of a LOAEL.) Source and date: IRIS, Last revised 03/01/1988</p> <p>Tier 2 Sources: PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per EPB-CCD/RRD, RfD = 8.3E-4. See Part 201 Value RfD details. Per CCD/WRD, RfD DEQ-SWQ RfD is based on an oral rat and mice feed study (https://ntp.niehs.nih.gov/ntp/htdocs/st_rpts/tox006.pdf) See EPB-CCD. RfD = 0.0017 ppm Critical Study: NTP, 1991. Toxicity Studies of pentachlorobenzene in F344/N rates and B6C3F1 mice. NTP TOX 6 NIH Publication No. 91-3125. Methods: Male mice (10/dose) were exposed to 0, 33, 100, 330, 1000, 2000 ppm pentachlorobenzene in diet for 13-weeks.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Critical effect: liver lesions End point or Point of Departure (POD): LOAEL = 33 ppm (5.2 mg/kg/day) Uncertainty Factors: UF = 3000 (10 each for intra-species variability, interspecies extrapolation, and use of a subchronic study and 3 for use of a LOAEL) Source and date: CCD-MDEQ/WRD, 6/18/2002</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day) ⁻¹	--	NA	MDEQ, 2015	
CSF details		<p>Carcinogen Weight-of-Evidence (WOE) Class: Class D; not classifiable as to human carcinogenicity IRIS WOE Basis: No human data and no animal data available Source and Date: IRIS; 2/1/1995;</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (2/1/1995), no value at this time PPRTV: No PPRTV record 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
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m ³)	--	1.0E-1	MDEQ, 2003	
RfC/ITSL details		<p>Tier 3 Source: MDEQ: Basis: MDEQ was the only value returned in the Tier 3 search. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS, no value at this time. PPRTV:] No PPRTV record available at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD/AQD (5/5/2003), ITSL = 0.1 µg/m³) based on a default value from R232 (1) (i).</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	
IURF details		<p>Carcinogen Weight-of-Evidence (WOE) Class: Class D; not classifiable as to human carcinogenicity WOE Basis: No human data and no animal data available Source and Date: IRIS; 2/1/1995;</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (date), no value at this time. PPRTV: No PPRTV record 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, 2015	
MMOA Details	--	<p>NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.</p>		
Developmental or Reproductive	--	No. The RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Effector? (Y/N)				
Developmental or Reproductive Toxicity Details	--	Per IRIS (3/1/1988); An acceptable daily intake (ADI) of 0.0167 mg/kg was reported in the 1980 Ambient Water Quality Criteria for Chlorinated Benzenes. This was based on the Khera and Villeneuve (1975) study dealing with reproductive effects of short-term (10-day) diet exposure in rats.		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	--	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	--	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 (A _{Ed})	---	0.1	MDEQ, 2015	
A _{Ed} details				
Ingestion Absorption Efficiency (A _{Ei})		0.5	MDEQ, 2015	
A _{Ei} 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 (M); 0.019
Updated GSI value (µg/L)	5 (M); 0.019
Rule 57 Drinking Water Value (µg/L)	5 (M); 0.38

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	0.38	6/2002
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	0.38	6/2002
Wildlife Value (WV)	0.019	6/2002
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)	1.2	6/2002
Aquatic maximum value (AMV)	11	6/2002
Final Acute Value (FAV)	21	6/2002

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 ($\mu\text{g}/\text{L}$)	5	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

