



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Pentachloronitrobenzene</b>
<b>CAS #:</b>	<b>82-68-8</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 16, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	295.32	295.34	EPI	EXP
<b>Physical State at ambient temp</b>	Solid	Solid	MDEQ	
<b>Melting Point (°C)</b>	419	144.00	EPI	EXP
<b>Boiling Point (°C)</b>	328	328.00	EPI	EXP
<b>Solubility (ug/L)</b>	32	440	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	0.002356	5.00E-05	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	2.90E-2	4.42E-05	PP	EST
<b>Log Kow (log P; octanol-water)</b>	4.64	4.64	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	36400	5996	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	2.63E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	6.92E-06	W9	EST
<b>Soil Water Partition Coefficient (Kd; inorganics)</b>	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 <sup>3</sup> )		1.718	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	1.69E-05	2.22E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	2.09E-05	2.22E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	2.19E-05	2.81E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	2.51E-05	2.81E-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>	7.5E-3	3.0E-3	IRIS, 1992	
<b>RfD details</b>	2-year feeding study in dogs; NOAEL = 0.75 mg/kg-d; UF = 100**; Critical effects = liver toxicity (Olin Mathieson Corp., 1968a). *RfD adjusted to two significant figures. **EPA uses an additional 3-fold factor to account for less than complete data base. CCD/RRD date: 4/15/87.	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is a Tier 1 source. IRIS RFD = 3.0E-3 mg/kg-day.  <b>Critical Study (ies):</b> Olin Mathieson Chemical Corporation. 1968a. MRID No. 00001667, 00083328, 00114201; HED Doc. No. 005188. Available from EPA. Write to FOI, EPA, Washington, DC 20460.  <b>Method(s):</b> Dogs (4 males and 4 females/group) were exposed to, 0, 30, 180, 1080 mg/kg/day in diet for 2-years.  <b>Critical effect:</b> Liver toxicity  <b>End point or Point of Departure (POD):</b> NOEL = 7.5E-1 mg/kg/day (30 ppm)  <b>Uncertainty Factors:</b> UF = 300; (10 each for intraspecies variability and interspecies extrapolation, and 3- for database deficiencies.  <b>Source and date:</b> IRIS; Last revision date - 1/1/1992. An EPA screening-level review in 2003 did not identify any critical new studies.</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD RRD (4/15/1978), RfD = 0.0075 mg/kg/day. See Part 201 value RfD details.</p>		Complete
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	--	NA	MDEQ, 2015	
<b>CSF details</b>		<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> D; not classifiable as to human carcinogenicity  <b>WOE Basis:</b> No human data and no animal data available.  <b>Source and Date:</b> IRIS, 2/01/1995</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (RfD revision date only 1/1/1992), no value at this time.  <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 (1/3/1993), no value at this time.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ( $\mu\text{g}/\text{m}^3$ )	5.0E+0	1.1E+1	MDEQ, 1992	
RfC/ITSL details	<p>Per AQD: ITSL is based on EPA's RfD value of 0.003 mg/kg/day. The critical study was conducted by Borzelleca et al. (1971) with the critical effect being liver toxicity. FINAL. AQD calculation date: 10/29/92.</p>	<p><b>Tier 3 Source:</b>  <b>MDEQ:</b>  <b>Basis:</b> MDEQ was the only value returned in the Tier 3 search. MDEQ value based on route extrapolated RfD value of 0.003 mg/kg/day. See details below.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (1/1/1992), no value at this time.  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b>  <b>Basis:</b> ITSL = 1.1E+1 <math>\mu\text{g}/\text{m}^3</math> is based on EPA's RfD value of 0.003 mg/kg/day.  <b>Critical Study:</b> Borzelleca et al. 1971. Toxicological and metabolic studies on pentachloronitrobenzene. <i>Toxicology and Applied Pharmacology</i>. 18: 522-534 (ecopy not available).  <b>Method:</b> animal: dogs (4 males and 4 females/group), duration: 2-years, doses: 0, 30, 180, 1080 mg/kg/day, and treatment: diet.  <b>Critical effect:</b> <u>liver toxicity</u>  <b>End point or Point of Departure (POD):</b> NOEL = 7.5E-1 mg/kg/day</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>Uncertainty Factors:</b> UF = 300; (10 each for intraspecies variability and interspecies extrapolation, and 3 for database deficiencies)</p> <p><b>Source and date:</b> MDEQ-CCD/AQD, 10/29/1992</p> <p><b>Other Tier 3:</b> 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, Canada, The Netherlands (RIVM), WHO (IARC), WHO (IPCS/INCHEM), ECHA (REACH), and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) (( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup> )	--	NA	MDEQ, 2015	
IURF details		<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> D; not classifiable as to human carcinogenicity</p> <p><b>WOE Basis:</b> No human data and no animal data available.</p> <p><b>Source and Date:</b> IRIS, 2/01/1995</p> <p><b>Tier 1 and 2 Sources:</b></p> <p><b>IRIS:</b> Per IRIS (RfD revision date only 1/1/1992), no value at this time.</p> <p><b>PPRTV:</b> Per PPRTV (date), RfD = [value] [OR] no value at this time. [OR] No PPRTV record available at this time.</p> <p><b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	<p>NA</p> <p>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 is not based on a reproductive-developmental effect.	MDEQ, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<b>State Drinking Water Standard (SDWS) (µg/L)</b>	--	NO	SDWA, 1976	
<b>SDWS details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (µg/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
<b>Is there an Aesthetic Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Aesthetic value details</b>	NA	NA		
<b>Is there a 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 (USEPA, 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>	NA
<b>Updated GSI value (µg/L)</b>	NA
<b>Rule 57 Drinking Water Value (µg/L)</b>	NA

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

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>	330	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	20	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	9.00E-01	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	3.00E+01	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