CHEMICAL UPDATE WORKSHEET

Chemical Name:	**1,3-Dichlorobenzene**
CAS #:	**541-73-1**
Revised By:	RRD Toxicology Unit
Revision Date:	September 16, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	147.01	147.00	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	---	-24.80	EPI	EXP
Boiling Point (˚C)	173	173.00	EPI	EXP
Solubility (ug/L)	1.11E+5	1.25E+05	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	2.3	2.15E+00	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	1.80E-3	2.63E-03	EPI	EXP
Log Kow (log P; octanol-water)	3.5	3.53	EPI	EXP
Koc (organic carbon; L/Kg)	708	375.3	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	5.58E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	8.8494E-06	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
Flash Point (˚C)	NA	72	CRC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		684.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		9.23E+03	EPA2004	EXP
Density (g/mL, g/cm^3)		1.2884	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	2.11E-05	2.58E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	3.42E-05	5.50E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	2.86E-05	4.02E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	4.26E-05	8.18E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	9.0E-4	2.0E-03	ATSDR 2006/MDEQ, 2015	
RfD details	RfD based on study by McCauley et al., 1995 (LOAEL 9 mg/kg UF=10,000). See file for review by Superfund health Risk Technical support Center Risk Assessment Issue paper #5 for 4th quarter 1998. CCD/RD date: 5/24/1999.	**Tier 2 Source:** **ATSDR:** **Basis:** ATSDR is a more recent assessment. MDEQ applied an additional UF (10x) to the intermediate MRL to account for subchronic to chronic exposure to derive a chronic oral RfD = 2.0E-3 mg/kg-day. The IRIS External review draft (2003) derived a chronic RfD = 1.0E-3 mg/kg-day based on the same study used by ATSDR; however ATSDR used a $BMDL_{10}$ as POD; IRIS used a BMDL value. The modified final MRL is preferred over the older draft IRIS value. **MRL:** Per ATSDR, no chronic oral MRL at this time. Intermediate oral MRL = 0.02 (2.0E-2) mg/kg-day based on endocrine effects: **Critical Study**: McCauley, P.T., M. Robinson, F.B. Daniel, and G.R. Olson (1995). Toxicity studies of 1,3-dichlorobenzene in Sprague-Dawley rats. Drug Chem. Toxicol. 18(2&3): 201-221. **Method(s)**: Groups of 10 male and 10 female Sprague-Dawley rats were administered 1,3-DCB in gavage doses of 0, 9, 37, 147, or 588 mg/kg/day in corn oil for 90 consecutive days. **Critical effect**: increased incidences of pituitary lesions, thyroid effects (reduced follicle colloidal density) **End point or Point of Departure (POD):** $BMDL_{10}$ = 2.1 mg/kg-d (BMDL based on increased pituitary lesions and basis of MRL) also noted: LOAEL = 9 mg/kg-d (thyroid lesions); 147 mg/kg-d (pituitary lesions); **Uncertainty Factors**: UF = 100 (10 each for intraspecies variability and interspecies extrapolation). Total UF = 1000 (included MDEQ applied UF) **Source and date:** ATSDR, 7/2006 **Tier 1 and 2 Sources**: **IRIS: Per IRIS (8/1/1992) no value.** IRIS is reassessing the toxicity of 1,3-DCB (external review draft – 11/03/2003). The reassessment derives an RfD = 1.0E-03		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		mg/kg-day based on the same sub-chronic oral gavage rat study used by ATSDR and MDEQ; however, the IRIS draft RfD used benchmark dose modeled value for its POD and a different total UF value. **Critical Study**: McCauley, P.T., M. Robinson, F.B. Daniel, and G.R. Olson (1995). Toxicity studies of 1,3-dichlorobenzene in Sprague-Dawley rats. Drug Chem. Toxicol. 18(2&3): 201-221. **Method(s)**: Groups of 10 male and 10 female Sprague Dawley rats were administered daily gavage doses of 0, 9, 37, 147, or 588 mg/kg of 1,3-dichlorobenzene in corn oil for 90 consecutive days **Critical effect**: thyroid and pituitary lesions **End point or Point of Departure (POD):** LOAEL = 9 mg/kg-d (thyroid lesions); 147 mg/kg-d (pituitary lesions); BMDL = 3 mg/kg-d **Uncertainty Factors**: UF = 3,000 (10 each for interspecies extrapolation, intraspecies variability and use of subchronic study and 3 for database deficiency). **Source and date:** IRIS external review draft, 11/03/2003 **PPRTV:** No PPRTV record available at this time **Tier 3 sources:** **MDEQ:** Per DEQ-CCD, RRD adopted HEAST RfD = 9.0E-4. See Part 201 Value RfD details.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	
CSF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: not classifiable as to human carcinogenicity (classification D) **IRIS WOE Basis**: no human data, no animal data and limited genetic data. **Source and Date**: IRIS, 9/01/1990; IRIS external review draft, 11/03/2003 **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/01/1990) and IRIS external review draft (2003), no value at this time. **PPRTV:** No PPRTV record available at this time.		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		MRL: NA; MRLs are for non-cancer effects only. **Tier 3 sources:** **MDEQ:** Per DEQ-CCD, no value at this time.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	3.0E+0	MDEQ, 2006	
RfC/ITSL details	NA	**Tier 3 Source:** **MDEQ:** **Basis:** MDEQ value is based on a 90-day oral toxicity study. The MDEQ and NYSDEC values and key study are the same. Documentation of the Texas value is not available. See details below. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (8/01/1992), no value at this time. **PPRTV:** No PPRTV record available at this time **MRL:** Per ATSDR (7/2006), no inhalation MRL at this time. **Tier 3 Sources:** **MDEQ-AQD:** ITSL = 3.0E+0 µg/m³ with an annual averaging time. This screening level is based on oral rat 90 day study (McCauley et al., 1995). Calculated using R232(1)(e) equation and default rat inhalation rate. **Critical Study**: McCauley, P.T., M. Robinson, F.B. Daniel, and G.R. Olson (1995). Toxicity studies of 1,3-dichlorobenzene in Sprague-Dawley rats. Drug Chem. Toxicol. 18(2&3): 201-221. **Method(s)**: Groups of 10 male and 10 female Sprague-Dawley rats were administered 1,3-DCB in gavage doses of 0, 9, 37, 147, or 588 mg/kg/day in corn oil for 90 consecutive days. **Critical effect**: thyroid pathology even at lowest dose tested **End point or Point of Departure (POD):** LOAEL = 9 mg/kg		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		Uncertainty Factors: UF = 3,000 (3 for LOAEL-to-NOAEL, 100 for inter-and intra-species extrapolation and 10 for subchronic to chronic exposure). **Source and date:** MDEQ-CCD/AQD, 8/02/2006 **New York DEC**: Per NYSDEC (2/2005) RfC = 10 µg/m³ based on exposure route extrapolation of the recommended oral RfD assuming a 70 kg adult and air breathing rate of 20 m^3/day. **Basis for RfD**: RfD of 3.0E-3 mg/kg-day from the USEPA Region 3 (20032; 2004; Draft). Per NYDEC, "value in online table is in error; correct value obtained via personal communication (USEPA Region 3, 2004)". **Critical Study**: McCauley, P.T., M. Robinson, F.B. Daniel, and G.R. Olson (1995). Toxicity studies of 1,3-dichlorobenzene in Sprague-Dawley rats. Drug Chem. Toxicol. 18(2&3): 201-221. **End point or Point of Departure (POD):** LOAEL = 9 mg/kg **Uncertainty Factors**: UF = 3000 (10 each for interspecies extrapolation, intraspecies variability, use of a LOEL, use of a subchronic study and 3 for database deficiency) **Source and date:** New York State Brownfield Cleanup Program, Development of Soil Cleanup Objectives: Technical Support Document, 2006, p.50. Table 5.1.1-2 Appendix A. **Texas CEQ:** RfC= 8.0E+0 µg/m³ (Source: NCEA). The NCEA document showing this value is not available. **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 and New Jersey, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: not classifiable as to human carcinogenicity (classification D)		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		IRIS WOE Basis: no human data, no animal data and limited genetic data. **Source and Date**: IRIS, 9/01/1990; IRIS external review draft, 11/03/2003 **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/01/1990) and IRIS external review draft (2003), no value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 sources:** **MDEQ:** Per DEQ-CCD, no value at this time.		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	Reported thyroid effects		
State Drinking Water Standard (SDWS) (ug/L)	--	NO	SDWA, 1976	
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		
Is there an aesthetic value for	NO	Not evaluated.	NA	

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
drinking water? (Y/N)				
Aesthetic value (ug/L)	NA	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 (ABSgi)	---	1.0	MDEQ, 2015/USEPA RAGS-E	
ABSgi details		RAGS E (EPA, 2004) Default Value		
Skin absorption efficiency value (AEd)	---	0.1	MDEQ, 2015	
AEd details				
Ingestion Absorption Efficiency (AEi)		1.0	MDEQ, 2015	
AEi 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)	28
Updated GSI value (µg/L)	28
Rule 57 Drinking Water Value (µg/L)	37

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	37	9/2003
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	65	9/2003
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)	28	9/2003
Aquatic maximum value (AMV)	100	9/2003
Final Acute Value (FAV)	200	9/2003

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 (μg/kg)	100	MDEQ, 2015
Target Detection Limit – Water (μg/L)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	4.90E-01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	1.60E+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