



CHEMICAL UPDATE WORKSHEET

Chemical Name:	3,3'-Dichlorobenzidine
CAS #:	91-94-1
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)	253.1	253.13	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	405	132.00	EPI	EXP
Boiling Point (°C)	368	368.00	EPI	EXP
Solubility (ug/L)	3110	3.1E+03	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.0000002204	2.56E-07	PP	EST
HLC (atm-m ³ /mol at 25°C)	4.00E-9	4.00E-09	SSG	EXP
Log Kow (log P; octanol-water)	3.51	3.51	EPI	EXP
Koc (organic carbon; L/Kg)	721	3190	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.0194	4.75E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	6.74E-6	5.5478E-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; unit less)	NA	NA	NA	NA
Critical Temperature (K)		754.03	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		2.00E+04	EPA2001	EST
Density (g/mL, g/cm ³)		NA	NA	NA
EMSOFT Flux Residential 2 m (mg/day/cm ²)	5.08E-08	4.93E-08	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	5.08E-08	4.93E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	5.24E-08	5.57E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	5.24E-08	5.57E-08	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	--	7.3E-3	MDEQ, 1999; 2015	
RfD details	NA	<p>Tier 3 Source: MDEQ: Basis: MDEQ was the only value returned in the Tier 3 search. MDEQ-RRD applied an additional UF = 10 to account for database deficiencies based on current IRIS approach to derive a final RfD = 7.3E-3 mg/kg-day. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (8/01/1990), no value at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: DEQ/WRD RfD = 7.3E-2 mg/kg-day. MDEQ-RRD applied an additional UF = 10 to account for database deficiencies based on current IRIS approach to derive a final RfD = 7.3E-3 mg/kg-day. Critical Study: Tsuda H, Miyata Y, Murasaki G, Kinoshita H, Fukushima S, Ito N (1977) Synergistic effect of urinary bladder carcinogenesis in rats treated with N-butyl- N-(4-hydroxybutyl)nitrosamine, N-[4-(5-nitro-2-furyl)-2-thiazolyl]formamide, N-2-fluorenylacetamide and 3,3'-dichlorobenzidine. Gann, 68:183-192. Method(s): male Wistar rats (n=18) were exposed to 0 or 0.03% (15 mg/kg BW) 3,3' dichlorobenzidine in diet for 40 weeks. Critical effect: no evidence of histopathological effects in the bladder or liver. End point or Point of Departure (POD): NOAEL = 0.03% (15.0 mg/kg-day) Per WHO/CICAD (1998), the Tsuda et al. study has limited period of exposure, small number of animals, single sex, and limited histopathological examination. Uncertainty Factors: UF = 300 (10 each for intraspecies variability and interspecies extrapolation and 3 for use of subchronic study). Total UF= 3000 including MDEQ-RRD additional UF.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Source and date: MDEQ-CCD/WRD, 9/05/1997</p> <p>WHO: Per WHO-IPCS/INCHEM (1998), available data are inadequate for developing tolerable intakes based on non-carcinogenic effects.</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, Canada, The Netherlands (RIVM), WHO (IARC), WHO (IPCS/INCHEM), ECHA (REACH) and OECD HPV.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	8.0E-1	4.5E-1	IRIS, 1993	
CSF details	<p>Liver tumors occurred in female beagle dogs following treatment via gelatin capsules 3 times/week for 6 weeks then 5 times/week for up to 7.1 years (Stula, 1978). Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. Source: MDEQ-CCD/WRD date: 1/13/2000</p>	<p>Tier 1 Source:</p> <p>IRIS:</p> <p>Basis: IRIS is a Tier 1 source. IRIS (1993) CSF = 4.5E-1 (mg/kg-day)⁻¹</p> <p>Critical Study: Stula, E.F., H. Sherman, J.A. Zapp and J.W. Clayton. 1975. Experimental neoplasia in rats from oral administration of 3,3'-dichlorobenzidine, 4,4'-methylene-bis(2-chloroaniline), and 4,4'-methylene-bis(2-methylaniline). Toxicol. Appl. Pharmacol. 31: 159-176.</p> <p>Method(s): ChR-CD rats (50/sex/dose group) were exposed to 3,3'-dichlorobenzidine at 1000 ppm (50 mg/kg/day) in the diet for the duration of the study (average was 349 days for females and 353 for males).</p> <p>1) <i>Dose response data: Tumor Type</i> - mammary adenocarcinoma; <i>Test Species</i> - rat/ChR-CD, female; <i>Route</i> - diet</p> <p>2) <i>Extrapolation method:</i> Linearized multistage procedure, extra risk</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen</p> <p>IRIS WOE Basis: increased tumor incidences in rats, mice and dogs and additional support provided by positive evidence of genotoxicity and structural relationship to the known human bladder carcinogen benzidine</p> <p>Source and Date: IRIS, Last revision date - 7/01/1993. An EPA screening level review on July 2006 did not identify any significant new studies.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Tier 2 Sources: 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/WRD (2000), CSF = 8.0E-1. See Part 201 Value CSF details.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (8/01/1990), no value at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Inhalation Unit Risk Factor (IURF) ($(\mu\text{g}/\text{m}^3)^{-1}$)	4.8E-4	3.4E-4	CAL-OEHHA, 1988/2009	
IURF details	<p>Potency based on Stula et al 1978. Female dogs developed urinary bladder transitional cell carcinomas (5/5). Oral potency of 8.57 E-2 (mg/kg)-1 was converted to</p>	<p>Tier 3 Source CALEPA: Basis: CALEPA is a more recent evaluation than MDEQ. Minnesota and New Jersey are based on CALEPA. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (7/07/1993), no value at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	air value. CCD/AQD date: 10/4/1983	<p>Tier 3 Sources:</p> <p>MDEQ: Per DEQ-CCD/AQD (1983), IURF = $4.8E-4 (\mu\text{g}/\text{m}^3)^{-1}$: Basis: Potency based on oral potency of $8.57 E-2 (\text{mg}/\text{kg}\cdot\text{day})^{-1}$ converted to an air value. Critical Study: Stula, E.F., J.R. Barnes, H. Sherman, C.F. Reinhardt and J.A. Zapp. 1978. Liver and urinary bladder tumors in dogs from 3,3'-dichlorobenzidine. J. Environ. Pathol. Toxicol. 1(4): 475-490. Method(s): ChR-CD rats (50/sex/dose group) were exposed to 3,3'-dichlorobenzidine at 1000 ppm (50 mg/kg/day) in the diet for the duration of the study (average was 349 days for females and 353 for males). Source and Date: MDEQ-CCD/AQD, 10/4/1983</p> <p>California EPA: Per OEHHA (2009), IURF= $3.4E-04 (\mu\text{g}/\text{m}^3)^{-1}$ calculated from a cancer potency factor of $0.21 (\text{mg}/\text{kg}\cdot\text{day})^{-1}$ derived in 1988). The extrapolation assumed a human breathing rate of $20 \text{ m}^3/\text{day}$, a human body weight of 70 kg, and 100% fractional absorption after inhalation exposure. The most sensitive experimentally determined endpoint for tumor development is mammary adenocarcinoma induction in female rats exposed to 3,3'-dichlorobenzidine (26/44 treated, 3/44 control) (Stula et al., 1975). Source and date: Technical Support Document for Describing Available Cancer Potency Factors. Appendix B, 2009, p. B-239. The CA value is from a more recent assessment than MDEQ.</p> <p>Minnesota PCA: IURF= $3.4E-04 (\mu\text{g}/\text{m}^3)^{-1}$ is based in CAL OEHHA value.</p> <p>New Jersey DEP: IURF= $3.4E-04 (\mu\text{g}/\text{m}^3)^{-1}$ is based in CAL OEHHA value.</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 Massachusetts, New York and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Mutagenic Mode of Action	--	NO	USEPA, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
(MMAO)? (Y/N)				
MMAO 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	NA		
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; 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 drinking water? (Y/N)	NO	Not evaluated.	NA	
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 (ABS _{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E	
ABS _{gi} details				
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)	0.3 (M); 0.2
Updated GSI value (µg/L)	0.3 (M,X); 0.2
Rule 57 Drinking Water Value (µg/L)	0.3 (M); 0.14

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	650	9/1997
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	950	9/1997
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	0.14	9/1997
Human Cancer values for non-drinking water source (HCV-Non-drink)	0.2	9/1997
Final Chronic Value (FCV)	4.5	10/1997
Aquatic maximum value (AMV)	41	10/1997
Final Acute Value (FAV)	81	10/1997

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 ($\mu\text{g}/\text{kg}$)	2,000	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	0.3	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