CHEMICAL UPDATE WORKSHEET

Chemical Name:	**Ethylene dibromide (1,2-Dibromoethane)**
CAS #:	**106-93-4**
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	187.9	187.86	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	283	9.90	EPI	EXP
Boiling Point (˚C)	131.6	131.60	EPI	EXP
Solubility (ug/L)	4.20E+6	3910000	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	7.6	1.12E+01	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	4.60E-4	6.50E-04	EPI	EXP
Log Kow (log P; octanol-water)	1.75	1.96	EPI	EXP
Koc (organic carbon; L/Kg)	52.5	39.6	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	4.30E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	1.04E-05	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)		583.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		8.31E+03	EPA2004	EXP
Density (g/mL, g/cm^3)		2.1683	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	2.36E-05	2.61E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	4.61E-05	5.70E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	3.27E-05	4.09E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	6.07E-05	8.56E-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-3	IRIS, 2004	
RfD details	NA	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. IRIS (2004) RfD = 9E-3 mg/kg-day: **Tier 1 Source:** **IRIS, 2004. Critical Study**: National Cancer Institute (NCI). (1978) Bioassay of 1,2-dibromoethane for possible carcinogenicity. Bethesda, MD: National Cancer Institute. NTIS no. PB 288428). **Methods**: Osborne-Mendel rats (50/group) given 40 and 80 mg/kg-day 1,2-dibromoethane 5 days/week in corn oil by gastric intubation caused high treatment-related mortality (18/50 males and 20/50 females). After week 16, the treatment was discontinued and suspended for 13 weeks and then restarted at week 30. The surviving rats received the low-dose regimen. Time-weighted average low- and high-doses were 38 and 41 mg/kg-day for male rats, and 37 and 39 mg/kg-day for female rats **Critical effects**: liver peliosis, ***testicular atrophy*** and adrenal cortical degeneration. **End point or Point of Departure (POD):** LOAEL = 27 mg/kg-day **Uncertainty Factors**: UF = 3,000 (10 each intraspecies variability, interspecies extrapolation, use of a LOAEL, and database insufficiency. The overall UF is 10,000; however, the EPA recommended maximum UF of 3,000 was applied (U.S. EPA, 2002). **Source and date:** IRIS, Last revision date - 7/29/2004 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, WRD (7/25/2006) adopted the IRIS RfD. See Part 201 RfD		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		details.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	5.7E+1	2.0E+0	IRIS, 2004	
CSF details	Rat 49 to 61 week gavage bioassay (NCI, 1978). Squamous cell carcinoma of the forestomach in male rats. Modified linearized multistage procedure used to account for varying time on-study for low and high dose groups. Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. Entry date: 3/20/2000	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. IRIS (2004) CSF = 2.0E+0 (mg/kg-day)$^{-1}$: **Critical Study**: National Cancer Institute. (1978) Bioassay of 1,2-dibromoethane for possible carcinogenicity. Bethesda, MD: National Cancer Institute. NTIS no. PB 288428. **Methods**: Osborne-Mendel rats (50/sex/group) and B6C3F1 mice were exposed to 1,2-dibromoethane by gavage to male and female. Time-weighted average doses were 38 and 41 mg/kg-day for male rats, and 37 and 39 mg/kg-day for female rats, and 62 and 107 mg/kg-day, respectively, for mice of both sexes. Doses were converted to human equivalent doses on the basis of (body weight)$^{3/4}$ 1) *Dose response data*: *Tumor Type* - forestomach tumors, hemangiosarcomas, thyroid follicular cell adenomas or carcinomas; *Test Species* - rat/Osborne-Mendel, male; *Route* - oral (gavage) 2) *Extrapolation method*: adjusted tumor incidence using poly-3 procedure **Carcinogen Weight-of-Evidence (WOE) Class**: "likely to be carcinogenic to humans" **IRIS WOE Basis**: strong evidence of carcinogenicity in animals and inconclusive evidence of carcinogenicity in an exposed human population **Source and Date**: IRIS, Last revision date - 7/29/2004 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/RRD (3/20/2000), CSF =5.7E+1 (mg/kg-day)$^{-1}$. See Part 201 Value CSF		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		details. Per DEQ-CCD (7/2006), WRD adopted the IRIS value.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	9.0E+0	IRIS, 2004	
RfC/ITSL details	NA	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. IRIS (2004) RfC = 9.0E-3 mg/m^3: **Critical Study**: NTP (National Toxicology Program). (1982) Carcinogenesis bioassay of 1,2-dibromoethane (CAS No. 106-93-4) in F344 rats and B6C3F1 mice (inhalation study). NTP-80-28, NIH publication no. 82-1766; Available from National Technical Information Service, Springfield, VA; PB82-181710. **Methods**: Fischer 344 rats and B6C3F1 mice (50/sex/species/exposure groups) were exposed to 0, 10, or 40 ppm (0, 77, or 307 mg/m3) 1,2-dibromoethane for 6 hr./day, 5 days/week. High-exposure rats of both sexes and female mice exhibited high mortality, resulting in early termination (between 78 and 91 weeks) of these groups. The low exposure groups were not terminated until the end of the study (104-106 weeks). **Critical effect**: nasal inflammation **End point or Point of Departure (POD):** $BMCL_{10}$(HEC) = 2.8 mg/m^3 **Uncertainty Factors**: UF = 300 (3 for interspecies pharmacodynamics and 10 each for intraspecies variability and database deficiencies) **Source and date:** IRIS, Last revision date - 7/29/2004 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD (8/02/2004), AQD adopted the IRIS value.		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	2.2E-4	6.0E-4	IRIS, 2004	
IURF details	IUR based on male rat nasal tumors from an inhalation study (Wong et al 1982), calc'd by EPA in IRIS. CCD/RRD date: 10/16/1992	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. IRIS (2004) IURF = 6.0E-4 (µg/m^3)$^{-1}$: **Critical Study**: NTP (National Toxicology Program). (1982) Carcinogenesis bioassay of 1,2-dibromoethane (CAS No. 106-93-4) in F344 rats and B6C3F1 mice (inhalation study). NTP-80-28, NIH publication no. 82-1766; Available from National Technical Information Service, Springfield, VA; PB82-181710. **Methods**: The continuous concentrations averaged over 24 hours per day and 7 days per week, 10 x (6/24) x (5/7) = 1.8 ppm, and 40 x (6/24) x (5/7) = 7.1 ppm were used for the calculation of benchmark concentrations and inhalation cancer slope factors. In addition, EPA RfC methodology (U.S. EPA, 1994, 2002) was used to estimate human equivalent dose corresponding to the nasal (extra-thoracic) region. See IRIS for further details. • *Dose response data*: *Tumor Type* - nasal cavity (includes adenoma, adenocarcinoma, papillary adenoma, squamous cell carcinoma, and or/papilloma), hemangiosarcomas, mesotheliomas; *Test Species* - rat/Fischer 344, male; *Route* - inhalation • *Extrapolation method*: multistage model **Carcinogen Weight-of-Evidence (WOE) Class**: "likely to be carcinogenic to humans" **IRIS WOE Basis**: strong evidence of carcinogenicity in animals and inconclusive evidence of carcinogenicity in an exposed human population **Source and Date**: IRIS, Last revision date - 7/29/2004 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, WRD (7/2006) adopted the IRIS value.		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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-oral NO-inhalation. The RfD is based on several critical effects including a reproductive-developmental effect. MDEQ does not consider this substance a developmental toxicant at this time.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	**Critical effects**: liver peliosis**,** ***testicular atrophy*** and adrenal cortical degeneration. **Critical Study**: National Cancer Institute (NCI). (1978) Bioassay of 1,2-dibromoethane for possible carcinogenicity. Bethesda, MD: National Cancer Institute. NTIS no. PB 288428).		
State Drinking Water Standard (SDWS) (ug/L)	0.05	0.05	SDWA, 1976	
SDWS details	SDWA, 1976	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, 2015		
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	NO	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Phytotoxicity details	NA	Not evaluated.	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, 2004	
ABSgi details		RAGS E (USEPA, 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)	5.7 (X)
Updated GSI value (µg/L)	5.7 (X)
Rule 57 Drinking Water Value (µg/L)	0.17

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	250	7/2006
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	8,200	7/2006
Wildlife Value (WV)	NA	
Human Cancer Values for Drinking Water Source (HCV-drink)	0.17	7/2006
Human Cancer values for non-drinking water source (HCV-Non-drink)	5.7	7/2006
Final Chronic Value (FCV)	15	7/2006
Aquatic maximum value (AMV)	140	7/2006
Final Acute Value (FAV)	280	7/2006

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)	20	MDEQ, 2015
Target Detection Limit – Water (μg/L)	0.05	MDEQ, 2015
Target Detection Limit – Air (ppbv)	5.60E-03	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	1.90E-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