CHEMICAL UPDATE WORKSHEET

Chemical Name:	**bis(2-Ethylhexyl)phthalate (DD)**
CAS #:	**117-81-7**
Revised By:	RRD Toxicology Unit
Revision Date:	November 18, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	390.57	390.57	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	223	-55.00	EPI	EXP
Boiling Point (˚C)	384	384.00	EPI	EXP
Solubility (ug/L)	340	2.70E+02	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	0.00000646	1.42E-07	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	1.02E-7	1.02E-07	SSG	EXP
Log Kow (log P; octanol-water)	7.3	7.60	EPI	EXP
Koc (organic carbon; L/Kg)	1.50E+7	1.196E+05	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.0351	1.73E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	3.66E-6	4.1807E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	420 F	218	CRC	EXP
Lower Explosivity Level (LEL; unit less)	NA	0.003	PC	EXP
Critical Temperature (K)		806.00	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		1.60E+04	EPA2001	EXP
Density (g/mL, g/cm3)		0.981	CRC	EXP
EMSOFT Flux Residential 2 m ($mg/day/cm^2$)	1.31E-10	1.26E-08	EMSOFT	EST
EMSOFT Flux Residential 5 m ($mg/day/cm^2$)	1.31E-10	1.26E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m ($mg/day/cm^2$)	1.32E-10	1.42E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m ($mg/day/cm^2$)	1.32E-10	1.42E-08	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	1.9E-2	6.0E-2	ATSDR, 2002	
RfD details	Guinea pig subchronic to chronic dietary bioassay (1 year) (Carpenter et al., 1953); NOAEL = none; LOAEL = 19 mg/kg/day (0.04% of diet) UF= 1000. Critical effect = increased relative liver weight. Source: IRIS MDEQ-CCD date: 1/22/1986	**Tier 2 Source:** **ATSDR:** **Basis:** ATSDR critical study is more recent than the IRIS study and based on reproductive effects. ATSDR (9/2002) chronic oral MRL = 0.06 mg/kg-day. **Critical Study**: David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di (2-ethylhexyl) phthalate in rats. Toxicol Sci 55:433-443. **Method(s)**: F344 rats were fed a diet containing DEHP in concentrations of 0 ppm (80/sex), 100 ppm (50/sex), 500 ppm (55/sex), 2,500 ppm (65/sex) or 12,500 ppm (80/sex) for up to 104 weeks. Reported average daily doses based on food consumption were 0, 5.8, 29, 147, or 789 mg/kg/day in males and 0, 7.3, 36, 182, or 939 mg/kg/day in females. No indication immature animals were dosed. **Critical effect**: testicular toxicity in the male rats **End point or Point of Departure (POD):** NOAEL = 5.8 mg/kg /day **Uncertainty Factors**: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) **Source and date:** ATSDR, final 9/2002 from April 2015 MRL list. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (5/1/1991), RfD = 2.0E-2 mg/kg-day **Critical Study**: Carpenter, C.P., C.S. Weil and H.F. Smyth. 1953. Chronic oral toxicity of di (2-ethylhexyl) phthalate for rats and guinea pigs. Arch. Indust. Hyg. Occup. Med. 8: 219-226. **Methods**: Guinea pigs (23-24/dose group/sex) were administered 0.04% and 0.13% DEHP in feed for 1 year. **Critical effect**: increased relative liver weights **End point or Point of Departure (POD):** LOAEL = 0.04% (19 mg/kg /day) **Uncertainty Factors**: UF = 1,000 (10 each for intraspecies variability and interspecies extrapolation. The last 10 is for use of subchronic study and LOAEL)		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Source and date: IRIS, Last revision - 5/01/1991. **PPRTV:** No PPRTV record available at this time. **MRL:** ATSDR (9/2002) also derived an intermediate oral MRL = 0.1 mg/kg-day based on reproductive effects; UF = 100. **Critical Study**: Lamb JC, Chapin RE, Teague J, et al. 1987. Reproductive effects of four phthalic acid esters in the mouse. Toxicol Appl Pharmacol 88:255-269. **Method(s)**: CD-1 Swiss mice were exposed to DEHP in the diet at calculated doses of 0, 14, 140, and 420 mg/kg/day. A continuous breeding protocol was used in which 11-week-old mice were exposed during a 7-day premating period and subsequently as breeding pairs for 98 days. There were 20 breeding pairs in each exposed group and 40 pairs in the control group. The pairs were segregated at the end of the 98-day breeding period so that females could deliver the final litter. The F0 mice were therefore exposed for a maximum possible duration of 105 days. **Critical effect**: reproductive toxicity in the male and female mice. **End point or Point of Departure (POD):** NOAEL = 14mg/kg /day **Uncertainty Factors**: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, RRD's (1/22/1986) RfD (1.9E-2) differed from IRIS RfD as two significant figures are presented. Water Resources Division posted the same value as RRD (1/12/1997).		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	3.2E-3	1.4E-2	IRIS, 1993	
CSF details	2-year carcinogenicity bioassay in mice and rats fed DEHP in diet for 103	**Tier 1 Source:** **IRIS:** **Basis:** IRIS value is the only CSF available. **Critical Study**: IRIS is a tier 1 source. NTP (National Toxicology Program). 1982. Carcinogenesis bioassay of di-(2-ethylhexyl)phthalate (CAS No. 117-81-7) in F344		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	weeks. Significant dose-related increases in liver tumor responses in rats and mice of both sexed (NTP, 1982.) Revised species scaling factor, $(BWh/BWa)^{0.25}$, was applied for q* calculation. Class B2 Carcinogen; Liver cell tumors (Source: SWQD, 1/10/2000	rats and B6C3F, mice (feed study). NTP Tech. Rep. Ser. TR No. 217, NTP, Research Triangle Park, NC. **Method(s)**: 2-year carcinogenicity bioassay in mice and rats fed DEHP in diet for 103 weeks. 1) *Dose response data*: *Tumor Type* - hepatocellular carcinoma and adenoma; *Test Species* - Mouse/B6C3Fl, male; *Route* - diet 2) *Extrapolation method*: Linearized multistage procedure, extra risk **Carcinogen Weight-of-Evidence (WOE) Class**: B2; probable human carcinogen. **IRIS WOE Basis**: dose-related increases in liver tumor responses in rats and mice of both sexes. **Source and Date**: IRIS, Last revision – 2/01/1993 **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, CSF = 3.2E-3; see details under Part 201 Value.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	7.0E+1	MDEQ, 2014	
RfC/ITSL details	NA	**Tier 3 Source:** **MDEQ:** **Basis:** Tier 3 search did not identify any other RfC values. See MDEQ details below. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (1/31/1987), no value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** Per ATSDR (July, 2013), no inhalation MRL at this time.		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Tier 3 Source: **MDEQ:** Per DEQ-CCD/AQD (3/3/2014), ITSL = 70 µg/m^3. Used EPA oral RfD of 0.02 mg/kg/day based on the Carpenter et al. (1953) guinea pig subchronic oral bioassay LOAEL of 0.04% diet (19 mg/kg bw/day) based on increased relative liver weight. (See RfD section.) Annual averaging time. **Other Tier 3 Sources:** The Tier 3 search did not produce any RfC values for this chemical.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	4.43E-6	1.6E-6	MDEQ, 2014	
IURF details	Potency based on draft NCI report. Oral potency of 15.5 E-3 (mg/kg)-1 was converted to inhalation value. AQD calculation date = 12/2/81	**Tier 3 Source:** **MDEQ:** **Basis:** MDEQ IURF is selected because it was calculated most recently and uses the updated human species scaling factor. All Tier 3 values are based on the same rodent cancer bioassay and tumor data. See details below. **Carcinogen Weight-of-Evidence (WOE) Class**: B2; probable human carcinogen. **IRIS WOE Basis**: dose-related increases in liver tumor responses in rats and mice of both sexes. **Source and Date**: IRIS, 2/01/1993 **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (2/01/1993), 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 CCD/AQD (3/3/2014), IURF = (µg/m^3)$^{-1}$ (reported incorrectly in CCD i.e., the oral CSF of 5.7E-3 per mg/kg-day is reported instead of the IURF of 1.6E-6 per µg/m^3). **Basis:** Potency based on WRD oral potency (q*) of 0.005745 (mg/kg/day)-1. The		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		key study for DEHP is based on the incidence of hepatocellular incidence in male B6C3F1 mice (NTP, 1982) which EPA used in the IRIS database. EPA used a species scaling factor of 2/3 power to extrapolate from mice to humans, whereas, WRD used 3/4 power. WRD q* of 0.005745 was converted to an inhalation factor. **Critical Study**: NTP (National Toxicology Program). 1982. Carcinogenesis bioassay of di-(2-ethylhexyl) phthalate (CAS No. 117-81-7) in F344 rats and B6C3F, mice (feed study). NTP Tech. Rep. Ser. TR No. 217, NTP, Research Triangle Park, NC. **Source and Date**: MDEQ-CCD/AQD, 3/3/2014 **CA (OEHHA)**: reports an IURF of 2.4E-6 per µg/m^3 based on the same NTP study used by MDEQ. It does not appear that a species scaling factor was used. The data for hepatocellular carcinomas in male mice was used and human equivalent doses derived. The data was modeled and a human potency factor of 8.36E-3 per mg/kg-day calculated. It appears that CA did not use the updated species scaling factor. A unit risk value of 2.4E-6 per µg/m^3 was derived assuming a 70 kg average human body weight, 20 m^3/day human breathing rate, and 100% fractional absorption. **MN Soil Remediation Value Spreadsheet (Draft, 2015):** IURF of 2.4E-6 based on CALEPA 6/1/2009. **NJ DEP, Division of Air Quality:** IURF of 2.4E-6 µg/m^3 based on the CA value.		
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	YES-oral, the RfD is based on a reproductive- effect – See RfD notes (testicular toxicity in male rats). In addition, Lamb et al, demonstrated decreased reproduction in male and female mice with dosing started preconception in a continuous breeding study. DR-RfD = 0.1 mg/kg-day. Oral Exposure Pathways- Single Exposure	MDEQ, 2014	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Developmental or Reproductive Toxicity Details	NA	See above (RfD details).		
State Drinking Water Standard (SDWS) (ug/L)	6.0	6.0	SDWA, 1976	
SDWS details	MI Safe Drinking Water Act (SDWA) 1976 PA 399	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	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, 2004	
ABSgi details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (AEd)	---	0.1	MDEQ, 2015	
AEd details				
Ingestion Absorption Efficiency (AEi)		0.5	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)	25
Updated GSI value (µg/L)	14
Rule 57 Drinking Water Value (µg/L)	14

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	120	11/1997
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	160	11/1997
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	14	2/2014
Human Cancer values for non-drinking water source (HCV-Non-drink)	18	2/2014
Final Chronic Value (FCV)	ID* (14)	9/1998
Aquatic maximum value (AMV)	285	9/1998
Final Acute Value (FAV)	285	9/1998

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)	330	MDEQ, 2015
Target Detection Limit – Water (μg/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 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