



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Polybrominated biphenyls (DD)</b>
<b>CAS #:</b>	<b>67774-32-7</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
Molecular Weight (g/mol)	NA	627.58416	PC	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	0	NA	NA	NA
Boiling Point (°C)	---	72.00	PC	EXP
Solubility (ug/L)	1.66E+7	11	PC	EXP
Vapor Pressure (mmHg at 25°C)	0.00000000191	5.20E-08	PC	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	3.90E-6	NA	NA	NA
Log Kow (log P; octanol-water)	7.07	6.39	PC	EXP
Koc (organic carbon; L/Kg)	8.91E+6	NA	NA	NA
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.08	2.59E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	8.0E-6	3.03E-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; 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> )		NA	NA	NA
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	NA	NA	EMSOFT	NA
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	NA	NA	EMSOFT	NA
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	NA	NA	EMSOFT	NA
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	NA	NA	EMSOFT	NA

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
<b>Reference Dose (RfD) (mg/kg/day)</b>	4.3E-6	1.0E-2	ATSDR, 2004	
<b>RfD details</b>	<p>Per SWQD: A dietary LOAEL of 0.3 ppm (0.042 kg/kg bwt) was found in a 15 month study in Rhesus monkeys (Lambrecht et al., 1978). CAS 1/1995 &amp; calc date 4/1999. No PPRTV. 9/29/11CF. No IRIS record available at this time (9/27/11). Per EPA RSL (May, 2013), RfD is 7.0E-6 mg/kg-day; source is HEAST. (DR-7/24/13)</p>	<p><b>Tier 2 Source:</b>  <b>ATSDR:</b>  <b>Basis:</b> The ATSDR MRL is selected because it is based on a more current and comprehensive assessment of PBBs: Toxicological Profile for Polybrominated Biphenyls and Polybrominated Diphenyl Ethers (10/2004). Per ATSDR, intermediate- and chronic-duration oral MRLs were not derived because serious developmental and reproductive effects were observed in monkeys that had been exposed to PBBs for durations that spanned the intermediate and chronic categories at the lowest dose tested in the database. This dose (0.012 mg/kg/day) caused increased menstrual cycle duration and implantation bleeding after 6–7 months of exposure and fetal deaths (fetal abortion and stillbirth) after ≈1 year of exposure in monkeys, with surviving infants having decreased birth weight and decreased postnatal weight gain (Allen et al. 1978, 1979; Lambrecht et al. 1978). Additionally, weight loss occurred in the maternal monkeys. The 0.012 mg/kg/day serious LOAEL for developmental and reproductive effects is lower than the lowest less serious LOAELs for thyroid effects in rats (0.05 mg/kg/day) (Akoso et al. 1982b) and hepatic effects in guinea pigs (0.04 mg/kg/day) (Sleight and Sanger 1976). As the most sensitive effect seen following intermediate-duration oral exposure was a serious LOAEL, without an accompanying NOAEL, concern for serious developmental and reproductive toxicity following exposures of &lt;1 year therefore precludes deriving an MRL for intermediate-duration exposure. Derivation of an MRL for chronic oral exposure is similarly precluded by the serious developmental effect (stillbirth) that occurred following exposures exceeding 1 year in duration. The serious LOAEL in monkeys is lower than the lowest chronic dosages tested in other species (0.5 and 1.3 mg/kg/day in rats and mice, respectively) that caused decreased survival (NTP 1992).  <b>ATSDR MRL:</b> Acute MRL = 0.01 mg/kg-day for an unspecified hexabromo mixture (35355-01-8). No intermediate nor chronic oral MRL is available.  <b>Critical Study:</b> Allen-Rowlands CF, Castracane VD, Hamilton MG, et al. 1981. Effect</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>of polybrominated biphenyls (PBB) on the pituitary - thyroid axis of the rat. <i>Proc Soc Exp Biol Med</i> 166:506-514</p> <p><b>Methods:</b> Groups of 8–11 male rats were treated with 0, 1, 3, or 6 mg/kg/day doses of an unspecified mixture of PBBs in lecithin liposomes by gavage for 10 days. Plasma T4 was assayed on treatment days 10 and 20. Other end points were evaluated on treatment day 20; these included plasma TSH levels, 5-hour thyroid uptake of <sup>131</sup>I, incorporation of <sup>131</sup>I into monoiodotyrosine, diiodotyrosine, T3 or T4, amount of intrathyroidal iodide, thyroid and liver weights, and body weights. Differences between mean values for the measured parameters in the control and PBB-treated groups were analyzed with the Student's <i>t</i>-test, with a <i>P</i> value of 0.05 considered as statistically significant</p> <p><b>Critical effect:</b> decreased plasma T4 levels</p> <p><b>End point or Point of Departure (POD):</b> NOAEL = 1 mg/kg/day</p> <p><b>Uncertainty Factors:</b> UF = 100; 10-fold extrapolation from animal to human and 10-fold for human variability</p> <p><b>Additional data:</b> ATSDR (2004) indicates that intermediate-duration studies show that the thyroid is a target of PBBs showing a spectrum of effects, including decreases in serum T3 and T4 hormone, thyroid enlargement, effects in the follicular cells (e.g., reduced size, hyperplasia with columnar appearance, and papillary projections) and accumulation of colloid droplets (Akoso et al. 1982a, 1982b; Byrne et al. 1987; Gupta and Moore 1979; Kasza et al. 1978a; Norris et al. 1975a, 1975b, 1975c; NTP 1983; Sepkovic and Byrne 1984; Sleight et al. 1978).</p> <p><b>Source and date:</b> ATSDR Toxicological Profile, 10/2004</p> <p><b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> No IRIS file available at this time. <b>PPRTV:</b> No PPRTV record available at this time.</p> <p><b>Tier 3 Source:</b> <b>MDEQ; RfD = 4.2E-6 mg/kg-day:</b> <b>Critical Study:</b> Lambrecht, L. K., et al. (1978). Response of nonhuman primates to</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>a polybrominated biphenyl mixture. <i>Environmental Health Perspectives</i>. 23: 193-145.</p> <p><b>Method(s):</b> Seven adult female monkeys were exposed to 0.3 ppm PBBs (estimated to be equivalent to 0.013 mg/kg/d based on data presented in EPA, 1988), were bred after 6 months of exposure and were then continued on the treatment for a total of 15 months. 3 monkeys were exposed to 1.5 ppm (0.063 mg/kg/d) in their feed for 9 months, whereas, 1 male and 1 female monkey were exposed to 25 ppm (1.0 and 1.1 mg/kg/d, respectively) for 14 weeks.</p> <p><b>Critical effect:</b> Adult monkeys exposed to 0.3 ppm exhibited a weight loss of 7.4% and an increase in the length of their menstrual cycles. Two of the 7 animals had prolonged implantation bleeding. Two of the 7 pregnant females aborted their young, whereas 5 had live births. All experimental infants were smaller than the controls at birth and their rate of weight gain was reduced.</p> <p><b>End point or Point of Departure (POD):</b> LOAEL = 0.3 ppm (0.013 mg/kg/day).</p> <p><b>Uncertainty Factors:</b> UF = 3,000 (10 each for intraspecies variation, sub chronic to chronic and LOAEL to NOAEL extrapolation. An additional 3fold UF was used to extrapolate from developmental effects in primates to humans (consistent with the UF used by EPA (1999) to derive an RfD for Aroclor 1016). WRD HNV justification is dated 1/1/1995.</p> <p><b>Source and date:</b> WRD&amp;RRD/EPB-CCD, 4/1/1999</p> <p><b>NOTE:</b> EPA RSLs (January 2015) used RfD = 7.0E-6 mg/kg/day based on HEAST</p>		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	7.2E+0	7.2E+0	MDEQ, 2000	
<b>CSF details</b>	Per RRD: The slope factor is based on the incidence of hepatocellular adenomas and carcinomas in female B6C3F1	<p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b></p> <p><b>Basis:</b> The MDEQ CSF is selected because it is based on a more current WRD re-assessment of PBB than HEAST. New Jersey and Texas are based on HEAST. See details below.</p> <p><b>Carcinogen Weight-of-Evidence (WOE) Class and basis:</b> Per IPCS (1994), based on the US National Toxicology Program (NTP) data, possible correlations between</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	<p>mice exposed to Firemaster FF-1 via the diet for 2 years (NTP, 1993). Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. RD calculation date: 1/18/2000</p>	<p>carcinogenicity and toxicity in laboratory rodents (Hoel et al., 1988) and between carcinogenicity and in vitro genetic toxicity assays (Tennant et al., 1987; Benigni, 1989; Ashby &amp; Tennant, 1991) have been analyzed for a series of PBB chemicals including the FireMaster(R) mixture. <i>Results confirm that FireMaster(R) can be classified as a nongenotoxic (epigenetic) carcinogen (see also Loury et al., 1987; Williams et al., 1989).</i></p> <p><b>Source:</b> WHO-IPCS. Polybrominated biphenyls (EHC 152, 1994)</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available 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 Sources:</b>  <b>MDEQ:</b> Per DEQ-CCD/RRD and WRD, RfD = 7.2E+0 (mg/kg-day)<sup>-1</sup>  <b>Critical Study:</b> NTP Toxicology and Carcinogenesis Studies of Polybrominated Biphenyls (CAS No. 67774-32-7) (Firemaster FF-1(R)) in F344/N Rats and B6C3F1 Mice (Feed Studies). <a href="#">Natl Toxicol Program Tech Rep Ser.</a> 1993. Aug; 398:1-235  <b>Method(s):</b> F344 rats and B6C3F1 mice were exposed to Firemaster FF-1 via the diet during the following life stages: adult-only (0, 10, and 30 ppm PBBs in food for 2 years.) perinatal exposure only, and combined perinatal and adult exposure. Per DEQ-CCD; The slope factor is based on the incidence of hepatocellular adenomas and carcinomas in female B6C3F1 mice exposed to Firemaster FF-1 via the diet for 2 years (NTP, 1993). Revised species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation. (See WRD justification.)  <b>Source and Date:</b> MDEQ-WRD and RRD, 1/1/1995 and 1/18/2000 respectively.</p> <p><b>HEAST:</b> CSF= 8.9 (mg/kg-day)<sup>-1</sup> from HEAST Summary 1997: route – gavage, species/duration: rat/ 637 days, target – liver, cancer – carcinoma and neoplastic nodules.</p> <p><b>New Jersey DEP:</b> CSF= 8.9 (mg/kg-day)<sup>-1</sup> is the HEAST value (NJDEP - Toxicity</p>		



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Factors for Polybrominated Biphenyls)</p> <p><b>Texas CEQ:</b> CSF= 8.9 (mg/kg-day)<sup>-1</sup> is the HEAST value (TCEQ. Summary of Updates to the Tables Accompanying the Texas Risk Reduction Program (TRRP) Rule, 2014).</p> <p><b>Other Tier 3:</b> No value is available at this time from these Tier 3 sources/databases: NTP ROC, health and environmental agencies of California, Massachusetts, Minnesota and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m<sup>3</sup>)</b>	NA	NA	MDEQ, 2015	
<b>RfC/ITSL details</b>	No AQD entry in EPB-CCD (9/27/11). No PPRTV (11/22/11; 7/24/13).	<p><b>Tier 1 and 2 Sources:</b></p> <p><b>IRIS:</b> No IRIS file available at this time.</p> <p><b>PPRTV:</b> No PPRTV record available at this time.</p> <p><b>MRL:</b> ATSDR (final 10/2004), no inhalation value at this time.</p> <p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b> Per DEQ-CCD no value at this time.</p>		Complete
<b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b>	--	NA	MDEQ, 2015	
<b>IURF details</b>	No AQD entry in EPB-CCD (9/27/11). No PPRTV (11/22/11; 7/24/13).	<p><b>Tier 1 and 2 Sources:</b></p> <p><b>IRIS:</b> No IRIS file available at this time.</p> <p><b>PPRTV:</b> 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



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	<p style="text-align: center;"><b>NA</b></p> Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	--	YES-oral, the RfD is based on a reproductive-developmental effect. Oral Exposure Pathways- Full Term Exposure Not known for inhalation.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	--	<p><b>Critical Study:</b> Allen-Rowlands CF, Castracane VD, Hamilton MG, et al. 1981. Effect of polybrominated biphenyls (PBB) on the pituitary - thyroid axis of the rat. <i>Proc Soc Exp Biol Med</i> 166:506-514</p> <p><b>Critical effect:</b> decreased plasma T4 levels</p> <p><b>Additional data:</b> ATSDR (2004) indicates that intermediate-duration studies had shown that the thyroid is a target of PBBs showing a spectrum of effects, including decreases in serum T3 and T4 hormone, thyroid enlargement, and effects in the follicular cells. Animal studies found that exposure during pregnancy or lactation caused changes in thyroid hormone levels in the newborns and at high doses increases in prenatal death and structural birth defects. Per ATSDR, because the nervous system and thyroid are developing in the fetus and child, the effects of PBB on these systems <b>may be critical for exposure before and soon after birth</b>, i.e. the fetus and child are more susceptible.</p>		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/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?	NO	Not evaluated.	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(Y/N)				
<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> )		0.5	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>	ID
<b>Updated GSI value (µg/L)</b>	ID
<b>Rule 57 Drinking Water Value (µg/L)</b>	0.01 (M); 0.00013

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	0.00031	4/1999
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	0.00031	4/1999
<b>Wildlife Value (WV)</b>	NA	
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	0.00013	4/1999
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	0.00013	4/1999
<b>Final Chronic Value (FCV)</b>	NLS	
<b>Aquatic maximum value (AMV)</b>	NLS	
<b>Final Acute Value (FAV)</b>	NLS	

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>	50	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	0.01	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	NA	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	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