



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Decabromodiphenyl ether(DD)</b>
<b>CAS #:</b>	<b>1163-19-5</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 28, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	959.22	959.17	EPI	EXP
<b>Physical State at ambient temp</b>	Solid	Solid	MDEQ	
<b>Melting Point (°C)</b>	---	305.00	EPI	EXP
<b>Boiling Point (°C)</b>	425	530.00	EPI	EXP
<b>Solubility (ug/L)</b>	30	1E-01	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	0.000000000000431	4.67E-12	PP	EST
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	4.02E-5	1.19E-08	PP	EST
<b>Log Kow (log P; octanol-water)</b>	5.24	12.11	ChemIDplus	Est; Meylan, WM 1995
<b>Koc (organic carbon; L/Kg)</b>	1.42E+5	2.762E+05	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	1.89E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	4.7688E-06	W9	EST
<b>Soil Water Partition Coefficient (Kd; inorganics)</b>	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)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm <sup>3</sup> )		3.0	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	3.87E-07	1.27E-09	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	3.87E-07	1.27E-09	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	4.61E-07	1.30E-09	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	4.61E-07	1.30E-09	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.0E-2	7.0E-3	IRIS, 2008	
RfD details	<p>2-year feeding study in rats NOAEL=1.0 mg/kg/d UF=100; Critical effects = no adverse effects observed (Kociba et al., 1973).</p> <p>CCD date: 4/15/1994</p>	<p><b>Tier 1 Source:</b> <b>IRIS:</b> <b>Basis:</b> IRIS is the only available value. <b>Critical Study:</b> Viberg, H; Fredriksson, A; Jakobsson, E; et al. (2003) Neurobehavioral derangements in adult mice receiving decabromodiphenyl ether (PBDE 209) during a defined period of neonatal brain development. Toxicol Sci 76:112-120. <b>Methods:</b> Single dose gavage study in neonates mice; Male mice were given a single oral dose of BDE-209 (&gt;99% purity) in a fat emulsion on post-natal days (PND) 3, 10 or 19. The PDN 3 and 19 groups were administered 0, 2.22 or 20.1 mg/kg bw, while PND 10 mice received 0, 1.34, 13.4 or 20.1 mg/kg bw. <b>Critical effect:</b> Neurobehavioral effects (spontaneous behavior measuring locomotion, rearing, and total activity). <b>End point or Point of Departure (POD):</b> NOAEL = 2.2 mg/kg <b>Uncertainty Factors:</b> UF = = 300 (10 each for interspecies variability and interspecies extrapolation and 3 as a “dosing duration adjustment”) <b>Source and date:</b> IRIS, Last revision date = 6/30/2008. An IRIS Toxicological Review is available</p> <p><b>Tier 2 Sources:</b> <b>PPRTV:</b> No PPRTV record is available at this time. <b>MRL:</b> No MRL record is available at this time.</p> <p><b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, 04/15/1994 (CAS date). RfD = 1.0E-2 mg/kg-day. See Part 201 Value RfD details.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day) <sup>-1</sup>	--	7.0E-4	IRIS, 2008	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
CSF details	NA	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is the only available value.  <b>IRIS</b> (9/30/2008), CSF = 7.0E-4 (mg/kg-day)<sup>-1</sup>:  <b>Critical Study:</b> NTP (National Toxicology Program). (1986) Toxicology and carcinogenesis studies of decabromodiphenyl oxide (CAS No. 1163-19-5) in F344/N rats and B6C3F1 mice (feed studies). Public Health Service, U.S. Department of Health and Human Services; NTP TR 309.  <b>Methods:</b></p> <ol style="list-style-type: none"> <li>1) <i>Dose response data: Tumor Type</i> - Liver neoplastic nodules or carcinoma (combined); <i>Test Species</i> - Male F344/N rats; <i>Route</i> - Oral, diet</li> <li>2) <i>Extrapolation method:</i> Multistage model with linear extrapolation from the point of departure (LED12).</li> </ol> <p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> suggestive evidence of carcinogenic potential  <b>IRIS WOE Basis:</b> based on (1) no studies of cancer in humans exposed to decaBDE; (2) statistically significant increases in incidence of neoplastic nodules in the liver of low- and high-dose male rats and high-dose female rats; (3) significantly increased incidences of hepatocellular adenoma or carcinoma (combined) in male mice at the low dose and marginally increased incidences at the high dose; (4) not significantly increased incidences of hepatocellular adenoma or carcinoma (combined) in female mice; (5) slightly greater (but not statistically significant) incidences of thyroid gland adenomas or carcinomas (combined) in dosed male and female mice; (6) significantly increased incidences in male mice, at both doses, of follicular cell hyperplasia, considered by many as a precursor to thyroid tumors; and (7) an apparent absence of genotoxic potential.  <b>Source and Date:</b> IRIS, Last revision date = 6/30/2008. A Toxicological Review (2008) is available</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time.		
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>	3.5E+1	2.5E+1	MDEQ, 2008	
<b>RfC/ITSL details</b>	ITSL based on EPA's RfD from two year rat feeding study with doses of 0, 0.01, 0.1 and 1 mg/kg reported by Kociba et al 1975. NOAEL of 1 mg/kg used by EPA to calc the RfD of 0.01 mg/kg. The EPA RfD was converted to the ITSL following methods in R232(1)(b).	<b>Tier 3 Source:</b> <b>MDEQ:</b> <b>Basis:</b> MDEQ is chosen because of access to details. Details of ECHA are unknown. See details below.  <b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (6/30/2008), no value at this time. <b>PPRTV:</b> No PPRTV record is available at this time. <b>MRL:</b> No MRL record is available at this time.  <b>Tier 3 Sources:</b> <b>MDEQ:</b> Per CCD/AQD, ITSL = 2.5E+1 $\mu\text{g}/\text{m}^3$ . Annual averaging time. <b>Basis:</b> Based on EPA's RfD 2008. The EPA RfD was converted to the ITSL following methods in R232(1)(b): <b>RfD derivation:</b> <b>Critical Study:</b> Viberg, H; Fredriksson, A; Jakobsson, E; et al. (2003) Neurobehavioral derangements in adult mice receiving decabromodiphenyl ether (PBDE 209) during a defined period of neonatal brain development. Toxicol Sci 76:112-120. <b>Methods:</b> Single dose gavage study in neonates mice; Male mice were given a single oral dose of BDE-209 (>99% purity) in a fat emulsion on post-natal days (PND) 3, 10 or 19. The PDN 3 and 19 groups were administered 0, 2.22 or 20.1 mg/kg bw, while PND 10 mice received 0, 1.34, 13.4 or 20.1 mg/kg bw. <b>RfD:</b> 7.0E-3 mg/kg-day		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Source and date:</b> MDEQ-CCD/AQD, 6/30/2008</p> <p><b>ECHA 2014:</b> Derived no effect level (DNEL) = 70 mg/m<sup>3</sup>. No further details are available for this inhalation value. Last modified 10/25/2014.</p> <p><b>Other Tier 3:</b> 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, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), and OECD HPV.</p>		
<b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b>	4.0E-7	2.0E-7	MDEQ, 2008	
<b>IURF details</b>	<p>Based on NTP 1986 - 2 year rat and mouse feeding study found increased liver neoplastic nodules, hepatocellular carcinomas and hepatocellular adenomas. Q1* of 1.4E-3(mg/kg)-1 based on male rats neoplastic nodules and carcinomas.</p> <p>CCD/AQD - 1994</p>	<p><b>Tier 3 Source:</b>  <b>MDEQ:</b>  <b>Basis:</b> Tier 3 search produced no other values for IURF. See details below.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (6/30/2008), no value at this time.  <b>PPRTV:</b> No PPRTV record is 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 CCD/AQD, IURF = 2.0E-7 (µg/m<sup>3</sup>)<sup>-1</sup>:  <b>Basis:</b> Based on NTP 1986 - 2 yr. rat and mouse feeding study found increased liver preneoplastic hyperplasia, hepatocellular carcinomas and hepatocellular adenomas. The oral SF of 7E-4(mg/kg)-1 derived by use of LED12 was based on rats preneoplastic and carcinomas. The oral SF was converted to inhalation using 20 m<sup>3</sup> inhalation rates in a 70 kg person.  <b>Source and Date:</b> MDEQ-CCD/AQD, 6/30/2008</p> <p><b>Other Tier 3:</b> 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, WHO</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		(IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	YES - for both oral and inhalation, the RfD and ITSL/RfC are based on reproductive-developmental effects. Oral Exposure Pathways- Single Exposure Inhalation Exposure Pathways- Single Exposure	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	<p><b>Critical effect:</b> Neurobehavioral effects (spontaneous behavior measuring locomotion, rearing, and total activity).</p> <p><b>Critical Study:</b> Viberg, H; Fredriksson, A; Jakobsson, E; et al. (2003) Neurobehavioral derangements in adult mice receiving decabromodiphenyl ether (PBDE 209) during a defined period of neonatal brain development. Toxicol Sci 76:112-120.</p> <p><b>Methods:</b> Single dose gavage study in neonates mice; Male mice were given a single oral dose of BDE-209 (&gt;99% purity) in a fat emulsion on post-natal days (PND) 3, 10 or 19. The PDN 3 and 19 groups were administered 0, 2.22 or 20.1 mg/kg bw, while PND 10 mice received 0, 1.34, 13.4 or 20.1 mg/kg bw.</p>		
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, 2015	
SMCL details	NA	SDWA, 1976 and USEPA SMCL List, 2015		
Is there an aesthetic value for drinking water?	NO	Not evaluated.	NA	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(Y/N)				
<b>Aesthetic value (ug/L)</b>	NA	NA	NA	
<b>Aesthetic Value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	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>	NA
<b>Updated GSI value (µg/L)</b>	NA
<b>Rule 57 Drinking Water Value (µg/L)</b>	NA

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

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>	330	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	10	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	8.84E-01	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	2.95E+02	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