



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>t-Butylbenzene</b>
<b>CAS #:</b>	<b>98-06-6</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	November 30, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	134.22	134.22	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	---	-57.80	EPI	EXP
Boiling Point (°C)	169.1	169.10	EPI	EXP
Solubility (ug/L)	NA	2.95E+04	EPI	EXP
Vapor Pressure (mmHg at 25°C)	NA	4.85E-06	EPI	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	NA	3.09E-09	PP	EST
Log Kow (log P; octanol-water)	4.11	4.11	EPI	EXP
Koc (organic carbon; L/Kg)	11000	1001	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.08	2.56E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	8.0E-6	6.5684E-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)		1220.00	NA	NA
Enthalpy of Vaporization (cal/mol)		8.98E+03	NA	NA
Density (g/mL, g/cm <sup>3</sup> )		0.8665	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	NA	2.64E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	NA	5.87E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	NA	4.14E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	NA	8.90E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	1.1E-2	1.0E-1	PPRTV, 2012	
RfD details	<p>The database is insufficient to support development of an RfD for tert-butylbenzene. Per Superfund Technical Support Center guidance, the RfD for isopropylbenzene (cumene) will be used as a surrogate with the addition of a 10-fold uncertainty factor. Critical effect = increased average kidney weight. CCD/RRD date: 1/30/1997</p>	<p><b>Tier 3 Source:</b>  <b>PPRTV Screening Value:</b>  <b>Basis:</b> No chronic or subchronic toxicity data were identified for deriving a provisional RfD (p-RfD) for tert-butylbenzene. PPRTV Appendix A used the surrogate approach to derive a provisional screening value. Isopropylbenzene (cumene) was identified as appropriate surrogate for tert-butylbenzene based on chemical-class-specific information. Per PPRTV, the surrogate approach assumes that all attributes such as critical effect, POD, and all UFs of the surrogate chemical should be adopted for the chemical of concern (unless a different adverse effect was used). EPA considers Screening Value a Tier 3 source.  <b>PPRTV (11/28/2012) Screening Value = 1.0E-1 mg/kg-day.</b> The screening chronic p-RfD for butylbenzene = 1E-1 mg/kg-day and is based on the IRIS RfD for isopropylbenzene. See details for isopropylbenzene below.  <b>IRIS (1997) File for the Surrogate: Isopropylbenzene (cumene) RfD Basis:</b>  <b>Critical Study:</b> Wolf, MA; Rowe, VK; McCollister, DD; et al. (1956) Toxicological studies of certain alkylated benzenes and benzene: Experiments on laboratory animals. AMA Arch Ind Health 14(4):387–398.  <b>Method(s):</b> Groups of 10 female Wistar rats were administered 139 doses of cumene by gavage in olive oil at 154, 462, or 769 mg/kg-day over a 194-day period; 20 rats given olive oil served as controls  <b>Critical effect:</b> increased average kidney weight in female rats  <b>End point or Point of Departure (POD):</b> NOAEL = 154 mg/kg-day (adjusted to 110 mg/kg-day for continuous exposure)  <b>Uncertainty Factors:</b> UF = 1000 (10 each for intraspecies variability and interspecies extrapolation and 3 each for use of less than chronic-duration study and database deficiencies.  <b>Source and date:</b> PPRTV, 11/28/2012; Cumene - IRIS 8/1/1997</p> <p><b>Tier 1 and 2 Sources:</b></p>		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>IRIS:</b> No IRIS file available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b> Per DEQ-CCD, RfD = 1.1E-2 mg/kg-day based on surrogate RfD. See Part 201 Value RfD details 1997.</p> <p><b>Minnesota Dept. of Health 2015:</b> RfD = 1.0E-1 mg/kg/day. Based on PPRTV (2012) use of IRIS (1997) surrogate cumene. Same as PPRTV screening level.</p> <p><b>New York DEP 2006:</b> RfD = 0.1 mg/kg/day. Based on IRIS 1997 cumene surrogate. Same as PPRTV screening level.</p> <p><b>Texas CEQ:</b> RfD=4.0E-02 mg/kg-day based on surrogate IRIS (1997) RfD for cumene. Texas CEQ justification document as IRIS 1997 cumene RfD as 4.0E-2 mg/kg/day. Based on a <b>NOAEL of 154 mg/kg</b> in female rats. <b>Critical study:</b> Wolf, MA; Rowe, VK; McCollister, DD; et al. (1956) Toxicological studies of certain alkylated benzenes and benzene: Experiments on laboratory animals. AMA Arch Ind Health 14(4):387-398. <b>UF = 3000;</b> 10 for each human variability, subchronic to chronic, interspecies extrapolation, and 3 for lack of reproductive studies.  <b>Source:</b> Texas CEQ tables 11/2014; NCEA (1997) Risk assessment issue paper for: Derivation of provisional chronic RfDs for n-butylbenzene (CASRN 104-51-8), sec-butylbenzene (CASRN 135-98-8), tert-butylbenzene (CASRN 98-06-6), and n-propylbenzene (CASRN 103-65-1), dated 6/5/1997. IRIS replaced the RfD on 8/1/1997. Texas value will not be used by MDEQ.</p> <p><b>Other Tier 3 sources:</b> No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Massachusetts, New Jersey, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
<p><b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b></p>	<p>--</p>	<p>NA</p>	<p>MDEQ, 2015</p>	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
CSF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "Inadequate Information to Assess Carcinogenic Potential"</p> <p><b>IRIS WOE Basis:</b> Little or no pertinent information available to assess carcinogenic potential of tert-butylbenzene.</p> <p><b>Source and Date:</b> PPRTV, 11/28/2012</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available at this time.  <b>PPRTV:</b> Per PPRTV (11/28/2012), no value at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	4.0E-1	CALEPA, 2005	
RfC/ITSL details	NA	<p><b>Tier 3 Source:</b>  <b>CALEPA:</b>  <b>Basis:</b> Tier 3 California and New York value is the same. CALEPA value is preferred over the MDEQ ITSL basis of a "surrogate LD50". See details below.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available at this time.  <b>PPRTV:</b> Per PPRTV (11/28/2012), no value at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b> Per DEQ-CCD/AQD (2008), ITSL = 1.0E+1 µg/m³ with annual averaging time. Based on unpublished male rat oral LD50 of 3045 mg/kg reported by Hazleton (1982) in EPA's OTS 0571879. ITSL calculated using R232(1)(h).</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>Critical Study:</b> Hazelton Laboratories. (1982) Initial submission: Acute oral toxicity in rats using t butyl benzene (with cover letter dated 08/24/92). Hazelton Laboratories No. 88920010733. (Unpublished)</p> <p><b>Method(s):</b> Rats (strain not specified) (5/sex/dose group) were exposed orally to a single-dose of 1000-, 2000-, 3000-, 4000-, or 5000-mg/kg tert-butylbenzene (purity not reported). The method of oral administration was not specified. Animals were examined for 14 days for mortality, body-weight changes, and clinical signs of toxicity. Use of a control group was not specified in the report, and a statement of GLP compliance was not provided.</p> <p><b>End point or Point of Departure (POD):</b> LD50 = 3045 mg/kg for male rats PPRTV (11/28/2012) reported that besides weight loss that was noted earlier in the study, no other details were provided in the report and an LD50 value was not reported, possibly due to lack of mortality in treated animals.</p> <p><b>Source and date:</b> MDEQ-CCD/AQD, 12/30/2008</p> <p><b>California DTSC 2014 (CALEPA):</b> RfC= 0.4 mg/m<sup>3</sup> = 400 µg/m<sup>3</sup> is based on a route extrapolated RfD of 0.1 mg/kg-day of a surrogate chemical, isopropylbenzene (cumene) (PPRTV, 2012). Tox value recommendation 2/2005. See RfD derivation in Updated Value RfD details. Source: <a href="#">Cal Dept of Toxic Substances Control (DTSC) Office of Human and Ecological Risk (HERO), Revised 7/14/2014</a> (page 21, table 3).</p> <p><b>New York DEC:</b> RfC = 0.4 mg/m<sup>3</sup> = 400 µg/m<sup>3</sup>. Per <a href="#">NYSDEC (2006)</a>, the US EPA reference concentration for isopropylbenzene (400 mcg/m<sup>3</sup> (US EPA IRIS, 2004)) is the toxicity value recommended for use in the derivation of an inhalation non-cancer-based soil cleanup objective for tert-butylbenzene. Same as CALEPA.</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 Massachusetts, Minnesota, New Jersey and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
<p><b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b></p>	<p>--</p>	<p>NA</p>	<p>MDEQ, 2015</p>	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
IURF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "Inadequate Information to Assess Carcinogenic Potential"</p> <p><b>IRIS WOE Basis:</b> Little or no pertinent information available to assess carcinogenic potential of tert-butylbenzene.</p> <p><b>Source and Date:</b> PPRTV, 11/28/2012</p> <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> Per PPRTV (11/28/2012), no value 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
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	<p>NA</p> <p>Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.</p>		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD or RfC 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 and USEPA SMCL List	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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 Exposure 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 (A <sub>Ed</sub> )	---	0.1	MDEQ, 2015	
A <sub>Ed</sub> details				
Ingestion Absorption Efficiency (A <sub>Ei</sub> )		1.0	MDEQ, 2015	
A <sub>Ei</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>	ID

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	ID	9/2010
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	ID	9/2010
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	NA	NA
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	NA	NA
<b>Final Chronic Value (FCV)</b>	ID	9/2010
<b>Aquatic maximum value (AMV)</b>	ID	9/2010
<b>Final Acute Value (FAV)</b>	ID	9/2010

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)



**(E) Analytical Information**

	<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>	1	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	1.80E+00	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	6.00E+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 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