



CHEMICAL UPDATE WORKSHEET

Chemical Name:	sec-Butylbenzene
CAS #:	135-98-8
Revised By:	RRD Toxicology Unit
Revision Date:	September 21, 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)	---	-82.70	EPI	EXP
Boiling Point (°C)	173.5	173.50	EPI	EXP
Solubility (ug/L)	NA	1.76E+04	EPI	EXP
Vapor Pressure (mmHg at 25°C)	NA	1.75E+00	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	NA	1.87E-02	CRC	EXP
Log Kow (log P; octanol-water)	4.57	4.57	EPI	EXP
Koc (organic carbon; L/Kg)	31100	1331	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.08	5.27E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.0E-6	7.32E-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	52	CRC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.008	CRC	EXP
Critical Temperature (K)		679.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		8.87E+04	EPA2004	EXP
Density (g/mL, g/cm ³)		0.858	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	2.65E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	5.93E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	4.16E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	9.02E-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 sec-butylbenzene. Per Superfund Technical Support Center guidance, the RfD of 1.1E-1 mg/kg/day for isopropylbenzene (cumene) will be used as a surrogate with the addition of a 10-fold uncertainty factor. Critical effect identified for cumene is increased average kidney weight. CCD-RD date: 1/30/1997.</p>	<p>Tier 3 Source: PPRTV Screening Value: Basis: PPRTV (11/28/2012) Screening Value = 1.0E-1 mg/kg-day is based on a surrogate (cumene) approach as no chronic or subchronic toxicity data were identified for the derivation of an oral provisional RfD. Per EPA, a Screening Value is a Tier 3 source. MDEQ (1997) and NCEA (1997) used the same approach but with a higher UF (10,000). PPRTV explains below why the UF of 3,000 was maintained. PPRTV (11/28/2012) Screening Value = 1.0E-1 mg/kg-day <u>Surrogate chemical:</u> Isopropylbenzene (cumene) was selected as the most appropriate surrogate chemical based on the weight of evidence: high similarity score, similar toxicokinetic profile and target organs, and comparable acute toxicity. The IRIS RfD for isopropylbenzene is 1.0E-1 mg/kg-day. Per PPRTV, “based on the current understanding of the surrogate approach, it is assumed that all attributes such as critical effect, POD, and all UFs of the surrogate chemical be adopted for the chemical of concern (unless a different [surrogate] adverse effect was used)”. <u>Isopropylbenzene RfD Derivation: RfD = 1.0E-1 mg/kg/day</u> Critical Study: 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. 062279 Method(s): 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 Critical effect: increased average kidney weight in female Wistar rat End point or Point of Departure (POD): NOAEL = 154 mg/kg-day (converted to 110 mg/kg-day for continuous exposure) Uncertainty Factors: UF = 1000 (10 each for intraspecies variability and interspecies extrapolation and 3 each for use of subchronic study and database</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>deficiencies).</p> <p>Source and date: IRIS, 8/1/1997</p> <p>Tier 1 and 2 Sources: IRIS: IRIS file for cumene surrogate (8/1/1997) is available. MRL: No MRL record available at this time. PPRTV: Per PPRTV (11/28/2012), no chronic or subchronic p-RfD at this time. A screening value of 1.1E-1 mg/kg-day based on a surrogate chemical has been derived (see details above).</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD (1/30/1997), RfD =1.1E-2 mg/kg-day is based on a surrogate chemical’s IRIS RfD. The surrogate chemical, isopropylbenzene (cumene), RfD of 1.0E-1 mg/kg-day was modified by DEQ applying a 10-fold uncertainty factor. See Part 201 Value RfD details.</p> <p>California DTSC: RfD = 1.0E-01 mg/kg-day based on PPRTV, 2012.</p> <p>Minnesota PCA: RfD = 1.0E-01 mg/kg-day based on PPRTV, 2012.</p> <p>New York DEC: RfD = 1.0E-01 mg/kg-day based on RfD of a surrogate chemical, isopropylbenzene (cumene). Source: New York State Brownfield Cleanup Program, Development of Soil Cleanup Objectives: Technical Support Document, 2006, p.50. Table 5.1.1-2 Appendix A p1.</p> <p>Texas CEQ: RfD= 4.0E-02 mg/kg-day is from NCEA (TCEQ, 2014).</p> <p>NCEA: Per NCEA (1997) the provisional RfD for sec-butylbenzene is 1.0E-2 mg/kg-day based on the cumene toxicity endpoint. NCEA applied a total UF of 10,000 to the cumene NOAEL of 154 mg/kg-day to derive this value. The IRIS RfD for cumene (4.0E-2 mg/kg-day) used a total UF of 3,000.</p>		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Source: NCEA "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) (97-009/6-5-97).</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of Massachusetts and New Jersey, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: "Inadequate information to assess carcinogenic potential"</p> <p>WOE Basis: There is little or no pertinent information available to assess the carcinogenic potential of sec-butylbenzene.</p> <p>Source and date: PPRTV, 11/28/2012</p> <p>Tier 1 and 2 Sources:</p> <p>IRIS: No IRIS file available at this time.</p> <p>PPRTV: Per PPRTV (11/28/2012), no value at this time.</p> <p>MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source:</p> <p>MDEQ: 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, 2011	
RfC/ITSL details	NA	<p>Tier 3 Source:</p> <p>CALEPA:</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Basis: California and New York value of 4.0E+2µg/m³. This value is preferred over the MDEQ ITSL basis of a “surrogate LD50”. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (11/28/2012), no value at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: ITSL = 6.0E+0 µg/m³. Averaging time = annual. Basis: based on “surrogate LD50” of 2 g/kg from a Dow proprietary range finding study. Critical Study: Dow Chemical. 1987. Results of range finding toxicological tests on sec-butylbenzene. Dow Chemical, Midland, MI; 86870002172; OTS0515962. 597631). Method(s): Acute oral toxicity study: Four rats (strain and sex not mentioned) were orally dosed at 2 g/kg sec-butylbenzene in 10% solution in corn oil. Critical effect: slight weight loss; dose caused no deaths End point or Point of Departure (POD): surrogate LD50 = 2.0 g/kg 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. Source and date: MDEQ-CCD/AQD - 3/04/1994</p> <p>California DTSC (CALEPA): RfC = 4.0E+2 µg/m³ based on the surrogate toxicity value for cumene, Source: CALEPA OEHHA, Updated 2011</p> <p>New York DEC: Per NYSDEC (2006), RfC= 4.0E+2 µg/m³ based on the route extrapolated RfD of a surrogate chemical, isopropylbenzene (cumene). Source: New York State Brownfield Cleanup Program, Development of Soil Cleanup Objectives: Technical Support Document, 2006, p.50.</p>		



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		Table 5.1.1-2 Appendix A p1. Other Tier 3: 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.		
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	Carcinogen Weight-of-Evidence (WOE) Class: "Inadequate information to assess carcinogenic potential" PPRTV WOE Basis: There is little or no pertinent information available to assess the carcinogenic potential of sec-butylbenzene. Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (11/28/2012), no value at this time. MRL: NA; MRLs are for non-cancer effects only. Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.		Complete
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, the RfD or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard	--	NO	SDWA, 1976	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(SDWS) (ug/L)				
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		
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 (ABS _{gi})	---	1.0	MDEQ, 2015	
ABS _{gi} details				
Skin absorption efficiency value (AE _d)	---	0.1	MDEQ, 2015	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		1.0	MDEQ, 2015	
AE _i 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)	ID
Updated GSI value (µg/L)	ID
Rule 57 Drinking Water Value (µg/L)	ID

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	ID	11/2000
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	ID	11/2000
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	NA
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	NA
Final Chronic Value (FCV)	ID	7/2010
Aquatic maximum value (AMV)	ID	7/2010
Final Acute Value (FAV)	ID	7/2010

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 ($\mu\text{g}/\text{kg}$)	50	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.10E+00	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	3.60E+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

