



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Benzoic Acid
CAS #:	65-85-0
Revised By:	RRD Toxicology Unit
Revision Date:	August 14, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	122.1	122.12	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	---	122.40	EPI	EXP
Boiling Point (°C)	249.2	249.20	EPI	EXP
Solubility (ug/L)	3.50E+6	3.400E+06	EPI	EXP
Vapor Pressure (mmHg at 25°C)	1	7.00E-04	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	1.54E-6	3.81E-08	PP	EST
Log Kow (log P; octanol-water)	1.86	1.87	EPI	EXP
Koc (organic carbon; L/Kg)	0.6	16.55	EPI	EST
Ionizing Koc (L/kg)		0.6	SSG	EST
Diffusivity in Air (Di; cm ² /s)	0.0536	7.02E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	7.97E-6	9.7868E-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	121	CRC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		751.00	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		1.21E+04	EPA2001	EXP
Density (g/mL, g/cm ³)		1.2659	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.74E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	1.74E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	2.20E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	2.20E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	4.4	4.0E+0	IRIS, 1993	
RfD details	<p>Considered a GRAS substance (Generally Recognized as Safe). Daily per capita intake (0.9-34 mg) of benzoic acid and sodium benzoate (34-328 mg) not associated with reports of toxic effects to humans. Critical effects = no observed adverse effects. UF=1 * See IRIS printout for conversion factors. Calc date: 9/17/1987</p>	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS RfD = 4.0E+0 mg/kg-day: Critical Study: FDA (Food and Drug Administration). 1973. Evaluation of the Health Aspects of Benzoic Acid and Sodium Benzoate as Food Ingredients. DHEW, Washington, DC. Report No. SCOGS-7. NTIS PB-223837/6. Method(s): Daily per capita intakes of 0.9-34 mg for benzoic acid and 34-328 mg for sodium benzoate were estimated based on data regarding the amounts used as a food preservative. At these levels, there are no reports of toxic effects in humans. The upper ranges were considered NOAELs for benzoic acid and sodium benzoate. In the stomach, the ionized form of both compounds is absorbed rapidly and completely by the GI tract. Therefore, per IRIS, exposure to sodium benzoate is comparable to exposure to benzoic acid if molecular weight differences are corrected for; 328 mg sodium benzoate is equivalent to 278 mg benzoic acid. Adding 278 to the daily intake for benzoic acid of 34 mg yields a total of 312 mg benzoic acid. Without uncertainty factor, the RfD is 312 mg/day for a 70 kg human or 4.4 mg/kg/day (rounded to 4.0 mg/kg-day) Critical effect: No adverse effects observed End point or Point of Departure (POD): NOAEL = 34 mg/day Uncertainty Factors: UF = 0. A UF for intra-species variability was not applied. Per IRIS, "Although reactions to benzoate and structurally related compounds do occur, an uncertainty factor of 10 would be of little value to the sensitive individuals." Source and date: IRIS, Last revision date - 7/01/1993. An EPA screening-level review in August 2003 did not identify any critical new studies. Note: IRIS does not currently develop updated assessments for registered pesticides unless the registered pesticides also have non-pesticide uses. The IRIS</p>		Complete



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		<p>user is referred to OPP Reregistration Eligibility Decision (RED) documents prepared by the Office of Pesticide Programs for additional health assessment information.</p> <p>Tier 1 and 2 Sources: EPA/OPP: OPP chronic RfD or PAD is not available. A Margin of Exposure (MOE) = 100 is available: Critical Study(ies): 1) NTP, 1989. Benzyl alcohol 13-week study in rats. 2) MRID: 43025501. Becker, H. (1991) Embryo toxicity Study (Including Teratogenicity) with benzyl Benzoate in the Rat: Lab Project Number: 294952. RCC Research and Consulting Co. AG. 371 p. (unpublished) Critical effect: 1) decreased body weight, mortality and neurotoxicity signs, 2) decreased fetal body weight and increased incidence of wavy ribs End point or Point of Departure (POD): NOAEL = 400 mg ai/kg-day (NTP, 1989); NOAEL = 625 mg/kg-day Uncertainty Factors: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) Source and date: EPA/OPP Reregistration Eligibility Decision (RED) for Benzyl Benzoate, 6/26/2007; OPP Benzoic acid. Human Health Effects Scoping Document for the Registration Review Decision, 10/19/2010.</p> <p>PPRTV: PPRTV (3/29/2005) refers to IRIS RfD. A provisional subchronic RfD of 4E+0 mg/kg-day is derived by adopting the chronic p-RfD as a health protective estimate for subchronic exposure.</p> <p>MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Refer to Part 201 Value. DEQ-CCD/RRD RfD = 4.4 mg/kg/day</p>		
<p>Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹</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>Carcinogen Weight-of-Evidence (WOE) Class: D, not classifiable as to human carcinogenicity</p> <p>IRIS WOE Basis: no human cancer data and inadequate data from animal bioassays</p> <p>Source and Date: IRIS, Last revision date = 5/1/91. EPA screening-level review in August 2003 did not identify any critical new studies.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (5/01/1991), no value at this time. PPRTV: Per PPRTV (3/29/2005), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	--	7.0E-1	PPRTV, 2005	
RfC/ITSL details	NA	<p>Basis: PPRTV (3/29/2005) is a Tier 2 source, not tier 1 available. Subchronic pRfC = $2.0\text{E}-3 \text{ mg}/\text{m}^3$. MDEQ applied an additional UF of 3 for subchronic to chronic extrapolation to derive a provisional chronic RfC = $7.0\text{E}-4 \text{ mg}/\text{kg}\text{-day}$ ($7.0\text{E}-1 \mu\text{g}/\text{m}^3$). No PPRTV chronic RfC is available at this time. PPRTV is the only available information.</p> <p>Subchronic pRfC derivation: Critical study: IRDC (International Research and Development Corporation). 1981. 4-week subacute inhalation toxicity study of benzoic acid in rats with amendment. FYI Submission by Velsicol Chemical Corporation to Office of Toxic Substances, U.S. Environmental Protection Agency, Washington DC. (unpublished)</p> <p>Methods: Sprague-Dawley rats (10/sex/dose) were exposed to benzoic acid dust by whole body inhalation at target concentrations of 0, 0.02, 0.2, or 2.00 mg/L, 6 hours/day, 5 days/week for four weeks.</p>		Complete

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		<p>Critical effect: pulmonary effects Critical end-point or POD: LOAEL_{RAT} = 25 mg/m³; LOAEL_{ADJ} = 4.46 mg/m³; LOAEL_{HEC} = 1.9 mg/m³ Uncertainty Factors: UF = 1,000 (10 for intraspecies variability and 3 each for use of subacute study, use of LOAEL, interspecies extrapolation, and lack of developmental and reproductive data by the inhalation route). Source and Date: PPRTV, 3/29/2005</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS ((5/01/1991), no value at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: D, not classifiable as to human carcinogenicity IRIS WOE Basis: absence of human data and inadequate data from animal bioassays Source and Date: IRIS, Last revision date = 5/1/91. EPA screening-level review in August 2003 did not identify any critical new studies.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (5/01/1991), no value at this time. PPRTV: Per PPRTV (3/29/2005), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Mutagenic Mode of Action	--	NO	USEPA, 2014	



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
(MMOA)? (Y/N)				
MMOA Details	--	NA		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2014	
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		
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/USEPA RAGS-E, 2004	
ABS _{gi} details		RAGS E (USEPA, 2004) Default Value		
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)	NA
Updated GSI value (µg/L)	NA
Rule 57 Drinking Water Value (µg/L)	NA

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

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 ($\mu\text{g}/\text{kg}$)	3,300	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	50	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