CHEMICAL UPDATE WORKSHEET

Chemical Name:	**n-Butanol**
CAS #:	**71-36-3**
Revised By:	RRD Toxicology Unit
Revision Date:	September 16, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	74.14	74.12	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	183	-89.80	EPI	EXP
Boiling Point (˚C)	117.7	117.70	EPI	EXP
Solubility (ug/L)	7.40E+7	6.32E+07	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	6.536	6.70E+00	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	8.81E-6	8.81E-06	EPI	EXP
Log Kow (log P; octanol-water)	0.851	0.88	EPI	EXP
Koc (organic carbon; L/Kg)	5.65	3.471	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	9.00E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	9.6E-6	1.0098E-05	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	84 F	37	CRC	EXP
Lower Explosivity Level (LEL; unitless)	0.014	0.014	CRC	EXP
Critical Temperature (K)		563.05	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		1.03E+04	EPA2001	EXP
Density (g/mL, g/cm3)		0.8095	CRC	EXP
EMSOFT Flux Residential 2 m ($mg/day/cm^2$)	1.51E-05	2.07E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m ($mg/day/cm^2$)	1.72E-05	3.09E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m ($mg/day/cm^2$)	1.91E-05	3.03E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m ($mg/day/cm^2$)	2.05E-05	4.03E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	1.3E-1	1.0E-1	IRIS, 1990	
RfD details	Rat oral sub chronic study. Critical effects = hypoactivity and ataxia. NOAEL = 125 mg/kg/d; UF = 1000 (US EPA, 1986); *EPA RfD adjusted to 2 significant figures. Source: IRIS MDEQ-CCD date: 5/14/1986	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available source that presents a value. **Critical Study**: U.S. EPA. 1986. Butanol: Rat oral sub chronic toxicity study. Office of Solid Waste, Washington, DC. (unpublished) **Method(s)**: Rats (30/sex/group) were dosed daily by gavage with 0, 30, 125 and 500 mg/kg/day of butanol for 13 weeks **Critical effect**: Ataxia and hypoactivity **End point or Point of Departure (POD):** NOAEL = 125 mg/kg-day **Uncertainty Factors**: UF = 1,000 (10 each for interspecies variability, interspecies extrapolation, and use of sub chronic study) **Source and date:** IRIS, Last revision date - 9/01/1990. An EPA screening-level review in 2003 did not identify any critical new oral studies. **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, RRD adopted IRIS value and adjusted it to 2 significant figures. Refer to Part 201 Value RfD details.		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	
CSF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: not classifiable as to human carcinogenicity **IRIS WOE Basis**: No human or animal cancer data are available. An IRIS screening-level review conducted in 2003 did not identify any critical new studies. **Source and Date**: IRIS, 9/01/1990		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Tier 1 and 2 Sources: **IRIS:** Per IRIS (3/01/1991), no value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, no value at this time.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	3.5E+2	3.5E+2	MDEQ, 1992	
RfC/ITSL details	ITSL based on EPA's RfD of 0.1 mg/kg. Study was unpublished EPA contracted 13 week rat gavage study, NOAEL of 125 mg/kg. DEQ-CCD/AQD date: 7/22/1992	**Tier 3 Source:** **MDEQ:** **Basis:** MDEQ value based on a route to route extrapolation of the IRIS RfD. Values published by Minnesota and Massachusetts did not have supporting information. ECHA (REACH) value is based on skin irritation endpoint although inhalation studies are available. See details below. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (3/01/1991), no value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Sources:** **MDEQ:** AQD (1992) ITSL = 3.5E+2 µg/m³, averaging time = 24 hours **Basis:** The EPA RfD (1.0E-1 mg/kg-day) was converted to an inhalation value. Refer to Updated Value RfC/ITSL details. Averaging time = 24 hours. **Study**: EPA. 1986. Butanol: rat oral sub chronic study. EPA, Office of Solid Waste, Washington DC. TRI #032-006. **End point or Point of Departure (POD):** NOAEL = 125 mg/kg, 500 mg/kg, caused reductions of hematological parameters, ataxia and hypoactivity		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Uncertainty Factors: UF = 1,000 (10 each for interspecies variability, interspecies extrapolation, and use of sub chronic study) **Calculation:** ITSL = (0.l mg/kg) x (70kg/20m^3) = 350 ug/m^3 **Source and date:** MDEQ-AQD, 7/22/1992 **Minnesota PCA**: RfC= 360 µg/m³. This Non-Cancer Chronic Air Concentration Value is listed in the "Toxicity Values (ug/m3) Used by MPCA for Air Toxics Comparisons". No information on source of value; however, the Remediation SRV Spreadsheet Draft 2015 does not include n-Butanol. **Massachusetts:** RfC= 412 µg/m³. This value comes from Massachusetts Air Guidelines Table, 2015 but there is not any additional information on the methods it was derived from. Source: Massachusetts Air Guidelines Table, 2015. **ECHA (REACH):** Derived No Effect Level (DNEL) = 55 mg/m^3 (5.5E+4 µg/m³). Most sensitive endpoint: skin irritation/corrosion Overall assessment factor (AF): 6 Derivation of the DNEL is not specified. Subs Key inhalation study: David, R.M., Tyler, T. R., Ouellette, R., Faber, W.D., Banton, M. I., Garman, R.H., Gill, M.W. and O'Donoghue, J.L. 2001. Evaluation Of Sub chronic Toxicity of n-Butyl Acetate Vapor. Fd. Chem. Toxicol. 39: 877-886, 2001. Methods: Sprague-Dawley rats (15/sex/dose) were exposed to 0, 500, 1500 and 3000 ppm (ca. 0, 2.35, 7.05 and 14.1 mg/L) by whole body inhalation (vapor) for 6 hrs., 5 days/wk., for 13 weeks (65 exposure days) Endpoint: NOAEL – 2.35 mg/L air (500 ppm) Critical effects: reduced body weight, food consumption and transient CNS effects; signs of necropsy of the olfactory epithelium Subs supporting study: David, R.M., Tyler, T. R., Ouellette, R., Faber, W.D., Banton, M. I., Garman, R.H., Gill, M.W. and O'Donoghue, J.L . 1998. Evaluation Of Sub chronic Neurotoxicity Of n-Butyl Acetate Vapor. Neurotoxicology 19: 809-822, 1998; cited in the OECD SIDS dossier 2008.		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM) and OECD HPV.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: not classifiable as to human carcinogenicity **IRIS WOE Basis**: No human or animal cancer data are available. An IRIS screening-level review conducted in 2003 did not identify any critical new studies. **Source and Date**: IRIS, 9/01/1990 **Tier 1 and 2 Sources:** **IRIS:** Per IRIS (3/01/1991), no value at this time. **PPRTV:** No PPRTV record available 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 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	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	NO	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 (ABSgi)	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABSgi details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (AEd)	---	0.1	MDEQ, 2015	
AEd details				
Ingestion Absorption Efficiency (AEi)		1.0	MDEQ, 2015	
AEi 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)	9,800 (X)
Updated GSI value (µg/L)	9,800 (X)
Rule 57 Drinking Water Value (µg/L)	3,500

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	3,500	7/2011
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	250,000	7/2011
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)	9,800	8/2011
Aquatic maximum value (AMV)	88,000	8/2011
Final Acute Value (FAV)	180,000	8/2011

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 (μg/kg)	4,400	MDEQ, 2015
Target Detection Limit – Water (μg/L)	800	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