CHEMICAL UPDATE WORKSHEET

Chemical Name:	**n-Butyl acetate**
CAS #:	**123-86-4**
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)	116.16	116.16	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	---	-78.00	EPI	EXP
Boiling Point (˚C)	125.5	126.10	EPI	EXP
Solubility (ug/L)	6.70E+6	8.400E+06	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	12.24	1.15E+01	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	3.20E-4	2.81E-04	EPI	EXP
Log Kow (log P; octanol-water)	1.78	1.78	EPI	EXP
Koc (organic carbon; L/Kg)	30.8	18.54	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	6.32E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	8.1221E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	72 F	22	CRC	EXP
Lower Explosivity Level (LEL; unitless)	0.017	0.017	CRC	EXP
Critical Temperature (K)		578	CRC	EXP
Enthalpy of Vaporization (cal/mol)		8.67E+03	CRC	EXP
Density (g/mL, g/cm3)		0.8825	CRC	EXP
EMSOFT Flux Residential 2 m ($mg/day/cm^2$)	1.64E-05	2.62E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m ($mg/day/cm^2$)	2.00E-05	5.72E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m ($mg/day/cm^2$)	2.13E-05	4.09E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m ($mg/day/cm^2$)	2.41E-05	8.60E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	7.6E-2	1.0E-1	WHO, 2005/ MDEQ, 2015	
RfD details	3-week rat inhalation study, LOAEL=1500 ppm; Critical effect = weight loss & decreased liver weight. UF=1000 (Hackett, 1983) adjusted for 7hrs/day, 5d/week. Source and date: DEQ-CCD/RRD 1/05/1994.	**Tier 3 Source:** **WHO:** **Basis:** The ECHA value is based on a route to route extrapolation of an inhalation value derived using a thirteen-week subchronic inhalation neurotoxicity study. The MDEQ value is based on a 3-week (gestation period) inhalation exposure. Texas CEQ (2001) value is based on a LD50. MDEQ used the recommended RfC of 0.4 mg/m^3 (WHO, 2005) to derive an oral RfD of 0.1 mg/kg-day assuming 80 kg body weight and 20 m^3/day air rate: RfD = (0.4 mg/m^3 x 20 m^3/day) / 80 kg = 0.1 mg/kg-day. See details below. **Tier 1 and 2 Sources**: **IRIS:** No IRIS file is available at this time. **PPRTV:** No PPRTV record is available at this time. **MRL:** No MRL record is available at this time. **Tier 3 Sources:** **MDEQ:** **Critical Study**: Hackett PL, Brown MG, Buschbom RL, Clark ML, Miller RA, Music RL, Rowe SE, Schirmer RE, Sikov MR (1983). Teratogenic study of ethylene and propylene oxide and n-butyl acetate. Springfield, VA, US Department of Commerce, National Technical Information Service (Report No. PB83-258038). **Method(s)**: female Sprague-Dawley rats (37-42) were exposed to 0 or 7260 mg/m^3 by inhalation for 3 weeks (5 days/week) prior to mating to untreated males and throughout days 1–16 of pregnancy. **Critical effect**: decrease in food intake and evidence of maternal toxicity (decreased body weights, decreased absolute liver weights, and increased relative kidney and lung weights) **End point or Point of Departure (POD):** LOAEL = 1500 ppm (adjusted for 7 hrs./day, 5 days/week)		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 LOAEL) **Source and date:** MDEQ-CCD/RRD, 1/05/1994. **Texas CEQ:** RfD = 1.4E-01 (mg/kg/day). Per TCEQ (4/25/2001), the value is derived as follows: Source: Hazardous Substances Data Bank POD: LD50 Rat oral 14.13 g/kg from The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 214 **PEER REVIEWED** LD50 = 14130 mg/kg Uncertainty Factors: 100,000 (10 each for acute to subchronic, subchronic to chronic, intraspecies variability, interspecies extrapolation, and database deficiencies) **ECHA (REACH):** Derived No Effect Level (DNEL) = 3.4 mg/kg/day. Oral DNEL is an extrapolation of the inhalation DNEL of 12 mg/m³. See Updated Value RfC details for inhalation DNEL derivation. **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, Massachusetts, Minnesota, New Jersey and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), and OECD HPV.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	
CSF details	NA	**Tier 1 and 2 Sources**: **IRIS:** No IRIS file available 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

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	7.1E+3	4.0E+2	WHO, 2005	
RfC/ITSL details	The ACGIH TLV has proposed adoption of the previous TLV value (713 mg/m3), which is consistent with the NIOSH value of 710 mg/m3. The ITSL was derived using the NIOSH OEL. CCD-AQD date: 4/3/98.	**Tier 3 Source:** **WHO:** **Basis:** The WHO (2005) value is selected as it is based on a thirteen-week subchronic inhalation neurotoxicity study in rat (Bernard and David, 1996 & Davis et al., 2001). MDEQ (1998) value is based on a NIOSH OEL. Texas CEQ (2012) and ECHA (REACH) values are also based on the same study but used different adjustment factors. **Tier 1 and 2 Sources**: **IRIS:** No IRIS file is available at this time. **PPRTV:** No PPRTV record is available at this time. **MRL:** No MRL record is available at this time. **Tier 3 Sources:** **MDEQ:** Per DEQ-CCD (4/3/1998), ITSL = 7.1E+3 µg/m³. Averaging time = 8 hr. **Basis:** The ITSL was derived using the NIOSH Occupational Exposure Limit (OEL) = 710 mg/m^3. Refer to Part 201 Value RfC details. **Source and date:** MDEQ-CCD/AQD, 4/03/1998 **Texas CEQ:** RfC = 4.7E+00 mg/m^3. TCEQ derivation: Key study: Bernard LG, RM David, RS Hosenfeld. 1996. n-Butyl acetate. A thirteen-week subchronic inhalation neurotoxicity study in the rat. As referenced in IPCS (2005). Method: Inhalation exposure of rats to 0, 500, 1,500, 3,000 ppm n-BA vapor Critical effects: transient sedation, reductions in body weight gain, olfactory lesions, and decreased transient motor activity (nervous system). The critical effects noted in rats are considered relevant to humans although, humans may be		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		less susceptible to the degeneration of olfactory epithelium (OECD 2001) because rats are obligate nose-breathers and the delivered dose to the olfactory epithelium is higher in rats than humans POD: NOAEL – 50 ppm. Supporting studies (David et al. 1998, 2001) reported the same NOAEL value as the key study. POD adjusted: 89.28 ppm PODHEC: 89.28 ppm UF: 90 (10 for intraspecies variability and 3 each for interspecies extrapolation and database insufficiency) Chronic REV: 990 ppb (4,700 µg/m³) Source: TCEQ Development Support Document for n-Butyl Acetate, 3/14/2014 **WHO (CICAD):** Tolerable concentration (TC) = 0.4 mg/m^3 (4.0E+2 µg/m³). **Basis:** Per WHO (2005), Tolerable Concentration (TC) = (2400 mg/m^3/1000) × (6/24) × (5/7) = 0.4 mg/m^3 **Critical Study:** 1) Bernard LG, David RM, Hosenfeld RS (1996) n-Butyl acetate. A thirteen-week subchronic inhalation neurotoxicity study in the rat. HAEL Nos. 93-0305 and 94-0306, KAN 900710, CAS No. 000123-86-4. Final report. Rochester, NY, Eastman Kodak Company, Corporate Health and Environmental Laboratories, Toxicological Sciences Laboratories (Laboratory Project Identification No. 93-030515). (unpublished); 2) David RM, Tyler TR, Ouellette R, Faber WD, Banton MI (2001) Evaluation of subchronic toxicity of n-butyl acetate vapor. Food and Chemical Toxicology, 39:877–886. **Method(s):** 13-week inhalation study in rats **Critical effect:** decreased growth, decreased transient motor activity (nervous system), and minimal to mild necrosis of the olfactory epithelium **End point or Point of Departure (POD):** NOAEC = 2400 mg/m^3 (exposure 6 h/day, 5 days/week) **Uncertainty Factors:** UF = 1,000 (10 each for interspecies variability, interspecies extrapolation, and use of subchronic study) **Source and date***:* Concise International Chemical Assessment Document 64: Butyl Acetates, WHO, 2005.		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		ECHA (REACH): Derived No Effect Level (DNEL) = 12 mg/m³ and 102.34 (mg/m³. These values are based on the same key study and NOAEC; however, the overall assessment factor (AF) applied are 50 and 1, respectively. Basis: Key study: (Bernard and David, 1996; David et al., 2001). Method: subchronic; male and female Sprague-Dawley rats (15 animals/sex/dose group) were exposed to nominal concentrations of 0, 500, 1500 or 3000 ppm of n-butyl acetate for 6 hours per day, 5 days per week for 13 consecutive weeks. The time-weighted average analytical concentrations were within 10% of the target concentrations. NOAEC: 500 ppm Critical effect: no systemic or organ-specific toxicity **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, Massachusetts, Minnesota, New Jersey and New York, WHO (IARC), Canada, The Netherlands (RIVM) and OECD HPV.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details	NA	**Tier 1 and 2 Sources**: **IRIS:** No IRIS file available 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.		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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	**A developmental study showed maternal effects. Further evaluation may be needed:** Critical Study: Hackett PL, Brown MG, Buschbom RL, Clark ML, Miller RA, Music RL, Rowe SE, Schirmer RE, Sikov MR (1983) Teratogenic study of ethylene and propylene oxide and n-butyl acetate. Springfield, VA, US Department of Commerce, National Technical Information Service (Report No. PB83-258038 Critical effect: decrease in food intake and evidence of maternal toxicity (decreased body weights, decreased absolute liver weights, and increased relative kidney and lung weights) Method(s): female Sprague-Dawley rats (37-42) were exposed to 0 or 7260 mg/m^3 by inhalation for 3 weeks (5 days/week) prior to mating to untreated males and throughout days 1–16 of pregnancy.		
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		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	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 (μg/kg)	250	MDEQ, 2015
Target Detection Limit – Water (μg/L)	10	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.50E+03	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	4.90E+04	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