



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>2-Butanone (MEK)(DD)</b>
<b>CAS #:</b>	<b>78-93-3</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	August 14, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	72.1	72.11	EPI	EXP
Physical State at ambient temp	Liquid	Liquid		
Melting Point (°C)	187	-86.60	EPI	EXP
Boiling Point (°C)	79.5	79.50	EPI	EXP
Solubility (ug/L)	2.40E+8	2.23E+08	EPI	EXP
Vapor Pressure (mmHg at 25°C)	91.2	9.06E+01	EPI	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	3.60E-5	5.69E-05	EPI	EXP
Log Kow (log P; octanol-water)	0.279	0.29	EPI	EXP
Koc (organic carbon; L/Kg)	1.99	4.51	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.081	9.14E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	9.8E-6	1.0193E-05	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	16 F	-9	CRC	EXP
Lower Explosivity Level (LEL; unit less)	NA	0.014	CRC	EXP
Critical Temperature (K)		536.78	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		7.48E+03	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.7999	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.15E-05	2.52E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	3.56E-05	5.18E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	2.91E-05	3.90E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	4.47E-05	7.56E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.8E+0	5.9E-1	IRIS, 2003	
RfD details	Rat multi-generation /development feeding study using the metabolic intermediate, 2-butanol, as surrogate for MEK. Critical effect = decreased fetal birth weight. NOAEL=1771 mg/kg/day; UF=1000. Source: MDEQ/RRD CCD date: 11/5/1992	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is the only value and a Tier 1 source.  <b>IRIS RfD</b> = 5.9E-1 mg/kg-day.  <b>Critical Study:</b> Cox, GE; Bailey, DE; Morgareidge, K. (1975) Toxicity studies in rats with 2-butanol (MEK) including growth, reproduction and teratologic observations. Food and Drug Research Laboratories, Inc., Waverly, NY. Report No. 91MR R 1673 (unpublished).  <b>Method(s):</b> weanling FDRL-Wistar stock rats (30/sex/group) were exposed to 0, 0.3, 1, or 3% 2-butanol in drinking water. After 8 weeks of initial exposure, F0 males and females from each group were mated to produce F1A litters, which were delivered naturally and nursed through 21 days of lactation. Because increased mortality and decreased body weight occurred in the F1A at the 3% dose level, all high-dose parents and F1A offspring were given drinking water without 2-butanol between days 10 and 21 of lactation and 2% 2-butanol for the remainder of the experimental protocol. After a 2-week post-lactation period, the F0 females were re-mated with males from their respective exposure group to produce F1B litters. The F1B pregnancies of 20 pregnant rats per group were terminated on gestation day 20. Selected male and female F1A rats (30/sex/group) were continued on their respective treatment protocols (0, 0.3, 1, or 2% 2-butanol) and mated at 12 weeks of age to produce F2 litters that were delivered and nursed through day 21 of lactation. F2 pup weights were assessed at days 4 and 21. Adult F1A rats were sacrificed at day 21.  <b>Critical effect:</b> Decreased pup (F1) body weight. The critical effect for MEK is based on its metabolic precursor, 2-butanol. Pharmacokinetic and toxicologic data support the use of 2-butanol as a surrogate for MEK.  <b>End point or Point of Departure (POD):</b> NOAEL = 594 mg/kg-day (0.3% 2-butanol solution) and the effective dose, LED<sub>05</sub> = 639 mg/kg-day  <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability, interspecies</p>	IRIS, 2003	Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		extrapolation and database deficiencies). <b>Source and date:</b> IRIS RfD was last revised 9/26/2003. An IRIS Toxicological Review is available.  <b>Tier 2 Sources:</b> <b>PPRTV:</b> No PPRTV record is available at this time. <b>MRL:</b> No MRL record is available at this time.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, RfD = 1.8E+0 mg/kg-day. See Part 201 Value RfD details.		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	--	NA	MDEQ, 2015	
<b>CSF details</b>	NA	<b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "data are inadequate for an assessment of human carcinogenic potential". <b>IRIS WOE Basis:</b> Studies of humans chronically exposed to MEK are inconclusive, and MEK has not been tested for carcinogenicity in animals by the oral or inhalation routes. <b>Source and Date:</b> IRIS, 9/26/2003  <b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (9/26/2003), no value at this time. <b>PPRTV:</b> No PPRTV record is available at this time. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time.		Complete
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m<sup>3</sup>)</b>	1.0E+3	5.0E+3	IRIS, 2003	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
<b>RfC/ITSL details</b>	Based on RfC, verified 7/17/91. ITSL of 1000 ug/m3 based on NOAEL of 2978 mg/m3 for decreased fetal birth weight in mice from Schwetz et al 1991 and Mast et al 1989. * Modified from IRIS. Extra 3-fold UF used by IRIS for incompleteness of the database. Source: AQD/EPA CCD date: 7/17/1991	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is the only value.  <b>IRIS RfC</b> = 5.0E+0 mg/m<sup>3</sup>.  <b>Critical Study:</b> Schwetz, BA; Mast, TJ; Weigel, R.J; et al. (1991) Developmental toxicity of inhaled methyl ethyl ketone in mice. Fund Appl Toxicol 16:742-748.  <b>Methods:</b> Mouse developmental study; Groups of 10 virgin Swiss CD-1 mice and 33 sperm plug-positive (gestation day 0) females were exposed to mean MEK concentrations of 0, 398±9, 1,010±28, or 3,020±79 ppm (0, 1,174±27, 2,980±83, or 8,909±233 mg/m3) by inhalation for 7 hours/day on gestation days 6-15. Dams were then sacrificed on gestation day 18.  <b>Critical effect:</b> developmental toxicity (skeletal variations)  <b>End point or Point of Departure (POD):</b> LEC = 5,202 mg/m<sup>3</sup>; LEC<sub>HEC</sub> = 1,517 mg/m<sup>3</sup>  <b>Uncertainty Factors:</b> UF = 300 (10 each for intraspecies variability and database deficiencies and 3 for interspecies extrapolation)  <b>Source and date:</b> IRIS, Last revision date - 9/26/2003</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> No PPRTV record is available at this time.  <b>MRL:</b> No MRL record is available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD (9/26/2003), AQD adopted IRIS RfC. Averaging time = 24hr.</p>		Complete
<b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b>	--	NA	MDEQ, 2015	
<b>IURF details</b>	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "data are inadequate for an assessment of human carcinogenic potential".  <b>IRIS WOE Basis:</b> Studies of humans chronically exposed to MEK are inconclusive, and MEK has not been tested for carcinogenicity in animals by the oral or inhalation routes.  <b>Source and Date:</b> IRIS, 9/26/2003</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (9/26/2003), no value at this time.  <b>PPRTV:</b> No PPRTV record is available 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>		
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	NO	USEPA, 2015	
<b>MMOA Details</b>	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
<b>Developmental or Reproductive Effector? (Y/N)</b>	Yes	YES-for both oral and inhalation, the RfD and RfC are based on reproductive-developmental effects. Oral Exposure Pathways- Full Term Exposure Inhalation Exposure Pathways- Single Exposure	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	<p><b>For RfD:</b>  <b>Critical effect:</b> Decreased pup (F1) body weight  <b>Developmental effect:</b> Decreased pup (F1) body weight  <b>Critical Study (ies):</b> Cox, GE; Bailey, DE; Morgareidge, K. (1975) Toxicity studies in rats with 2-butanol including growth, reproduction and teratologic observations. Food and Drug Research Laboratories, Inc., Waverly, NY. Report No. 91MR R 1673. (Unpublished). The critical effect for 2-butanone (MEK) is based on its metabolic precursor, 2-butanol, the surrogate chemical for MEK.</p> <p><b>For RfC:</b>  <b>Critical effect:</b> developmental toxicity (skeletal variations)  <b>Critical Study):</b> Schwetz, BA; Mast, TJ; Weigel, R.J; et al. (1991) Developmental toxicity of inhaled methyl ethyl ketone in mice. Fund Appl Toxicol 16:742-748.</p>		
<b>State Drinking Water Standard (SDWS) (ug/L)</b>	--	NO	SDWA, 1976	
<b>SDWS details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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		
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	
ABS <sub>gi</sub> details		RAGS E (EPA, 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>	2,200
<b>Updated GSI value (µg/L)</b>	2,200
<b>Rule 57 Drinking Water Value (µg/L)</b>	17,000

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	17,000	5/2010
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	1,300,000	5/2010
<b>Wildlife Value (WV)</b>	NA	
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	NA	
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	NA	
<b>Final Chronic Value (FCV)</b>	2,200	1/2010
<b>Aquatic maximum value (AMV)</b>	20,000	1/2010
<b>Final Acute Value (FAV)</b>	40,000	1/2010

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>	750	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	25	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	1.70E+03	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	5.60E+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