



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Isobutyl alcohol
CAS #:	78-83-1
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 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)	165	-108.00	EPI	EXP
Boiling Point (°C)	107.8	107.80	EPI	EXP
Solubility (ug/L)	7.60E+7	85000000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	10.64	1.05E+01	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	1.30E-5	9.78E-06	EPI	EXP
Log Kow (log P; octanol-water)	0.75	0.76	EPI	EXP
Koc (organic carbon; L/Kg)	5.46	2.919	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.08	8.97E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.0E-6	1.00E-05	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	82 F	28	CRC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.017	CRC	EXP
Critical Temperature (K)		547.78	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		1.09E+04	EPA2004	EXP
Density (g/mL, g/cm ³)		0.8018	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	1.69E-05	2.12E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	2.08E-05	3.25E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	2.18E-05	3.11E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	2.49E-05	4.27E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	3.0E-1	3.0E-1	IRIS, 1991	
RfD details	<p>Oral rat sub chronic toxicity study. High dose treatment resulted in a minor decrease in body weight gain during week 2 and decreased serum potassium levels and hypoactivity. NOAEL = 316 mg/kg/d. UF = 1,000 including 10 for use of sub chronic study. IRIS, 1991.</p>	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS oral RfD = 3.0E-1 mg/kg-day. Critical Study: U.S. EPA, 1986. Rat oral sub chronic toxicity study with isobutyl alcohol. Office of Solid Waste, Washington, DC. Method(s): 30 rats/sex/group were dosed daily with 0, 100, 316, and 1,000 mg/kg/day of isobutyl alcohol by oral gavage for 13 weeks. There were no effects on body weight or clinical and histopathologic parameters at doses less than or equal to 316 mg/kg/day. Treatment at the high dose resulted in minor decreases in body weight gain during week 2 and decreased serum potassium levels and hypoactivity. Hypoactivity was the most frequently observed clinical sign. Ataxia was also seen at low incidence in the high dose group throughout the study. Critical effect: Hypoactivity and ataxia. End point or Point of Departure (POD): NOEL = 316 mg/kg-day Uncertainty Factors: UF = 1,000 (10 for interspecies extrapolation, 10 for interspecies variability and 10 for extrapolating sub chronic exposure to chronic exposure). Source and date: IRIS, 04/01/1991.</p> <p>Tier 2 Sources: PPRTV: PPRTV (5/31/2002). Oral noncancerous effects have not been evaluated. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ-RRD: DEQ-CCD reports an oral RfD of 0.32 mg/kg/day (unrounded from the IRIS value of 3E-1 mg/kg/day) 5/14/1986. Rat oral sub chronic study. LOAEL = 1,000 mg/kg. Critical effects are hypoactivity and ataxia. NOAEL = 316 mg/kg; UF = 1,000 (EPA, 1986).</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	NA	NA	MDEQ, 2015	
CSF details		<p>Tier 1 and 2 Sources: IRIS: No cancer assessment in IRIS (1991). PPRTV (5/31/2002): Oral cancer effects have not been evaluated. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no oral cancer slope factor value available at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	1.5E+3	1.5E+3	MDEQ, 1996	
RfC/ITSL details	Per AQD: ITSL is based on NIOSH Recommended Exposure Limit (REL) of 150 mg/m ³ . NIOSH (1994) lists critical effects of eye/throat irritation and headache on inhalation exposure as the basis of the REL. 8 hr. averaging time. FINAL. AQD calculation date:	<p>Tier 3 Source: MDEQ: Basis: Details for the oral data used to extrapolate to an RfC by CA was not located on-line. MDEQ-AQD selected as the best available endpoint. See details below.</p> <p>Tier 1 and 2 Sources): IRIS: Per IRIS (4/1/1991), a chronic RfC is not available at this time. PPRTV: Per PPRTV (5/31/2002), the database is inadequate for deriving an RfC. There are no long-term studies in humans and limited studies in animals. MRL: No MRL record is available at this time.</p> <p>Tier 3 Source: MDEQ-AQD: Per DEQ-CCD, the AQD ITSL (1.5E+3 µg/m³) is based on the NIOSH recommended exposure limit (REL) of 150 mg/m³. NIOSH (1994) lists critical effects of eye/throat irritation and headache on inhalation exposure as the basis of the REL. 11/6/1996. The same is reported for MDEQ-RRD.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	11/6/96.	<p>California DTSC: RfC= 1.2E+03 ($\mu\text{g}/\text{m}^3$) based on a route to route extrapolation from an oral toxicity value using 80 kg body weight and 20 m^3 daily inhalation rate and a conversion factor of 1000 $\mu\text{g}/\text{mg}$. No further details are provided on-line.</p> <p>Massachusetts: RfC= NA; an Allowable Ambient Limit of 41.22 $\mu\text{g}/\text{m}^3$ and a Threshold Effects Exposure Limit (24 hour average) of 41.22 ($\mu\text{g}/\text{m}^3$) is also provided with no details about the toxicity endpoint used.</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, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ($(\mu\text{g}/\text{m}^3)^{-1}$)	NA	NA	MDEQ, 2015	
IURF details		<p>Tier 1 and 2 Sources: IRIS: No cancer assessment in IRIS (1991). PPRTV (5/31/2002): Inhalation cancer effects have not been evaluated. MRL: No MRL record is available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no IURF reported for either RRD or AQD.</p>		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	No	USEPA, 2015	
MMOA Details	--	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		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/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? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	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 ($\mu\text{g}/\text{kg}$)	4,400	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	1,000	MDEQ, 2015
Target Detection Limit – Air (ppbv)	4.90E+02	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	1.63E+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