CHEMICAL UPDATE WORKSHEET

Chemical Name:	**Diethylene glycol monobutyl ether**
CAS #:	**112-34-5**
Revised By:	RRD Toxicology Unit
Revision Date:	August 17, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	162.23	162.23	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	---	-68.00	EPI	EXP
Boiling Point (˚C)	230.6	231.00	EPI	EXP
Solubility (ug/L)	1.0E+9	1E+09	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	0.0219	2.19E-02	EPI	EXP
HLC (atm-m³/mol at 25˚C)	1.52E-9	7.20E-09	EPI	EXP
Log Kow (log P; octanol-water)	0.32	0.56	EPI	EXP
Koc (organic carbon; L/Kg)	2.06	10	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	4.14E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	6.9707E-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	78	PC	EXP
Lower Explosivity Level (LEL; unit less)	NA	0.008	PC	EXP
Critical Temperature (K)		692	CRC	EXP
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm^3)		0.9553	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	1.67E-06	1.04E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	1.67E-06	1.04E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	1.91E-06	1.30E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	1.91E-06	1.30E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	1.2E-2	3.0E-2	PPRTV, 2009	
RfD details	Sub chronic rat gavage study (Hobson et al; Naval Medical Research Institute). LOAEL = 50 mg/Kg-day*5/7 = 35.7, UF=3000; Lowest dose tested caused leukemia and one female death. Source: DEQ/ERD CCD date: 8/20/1992	**Tier 2 Source:** **PPRTV:** **Basis:** PPRTV is a tier 2 source, no tier 1 available. PPRTV p-RfD = 3.0E-2 mg/kg-day. **Critical Study**: Johnson, K.A., P.C. Baker, H.L. Kan et al. 2005. Diethylene glycol monobutyl ether (DGBE): Two- and thirteen-week oral toxicity studies in Fischer 344 rats. Food Chem. Toxicol. 43:467−481. **Method(s)**: F344 rats (10 rats/sex/dose group) were exposed to 0, 50, 250, or 1,000 mg/kg-day DGBE in drinking water daily for 13 weeks. **Critical effect**: reduced red blood cells count in male rats **End point or Point of Departure (POD):** $BMDL_{1SD}$ = 81 mg/kg-day **Uncertainty Factors**: UF = 3,000 (10 each for interspecies variability, interspecies extrapolation and use of a sub chronic study, and 3 for database deficiencies.) **Source and date:** PPRTV, 9/28/2009 **Tier 1 and 2 Sources**: **IRIS:** No IRIS file available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/RRD (8/20/1992), RfD = 1.2E-2 mg/kg-day. See 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**: "there is inadequate information to assess the carcinogenic potential" **IRIS WOE Basis**: No adequate information on the carcinogenicity of DGBE due to a lack of oral, inhalation, or dermal studies in animals longer than 13 weeks in duration. Genotoxicity testing of DGBE in vitro with bacteria and mammalian cells		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		and in vivo with Drosophila and mice have yielded negative results in all but one study. **Source and Date**: PPRTV, 9/28/2009 **Tier 1 and 2 Sources**: **IRIS:** No IRIS file available at this time. **PPRTV**: Per PPRTV (9/28/2009), no value 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)	2.0E+1	1.0E-1	PPRTV, 2009	
RfC/ITSL details	ITSL based on EPA's RfC. Source:AQD/EPA Entry date: 10/19/1992	**Tier 2 Source:** **PPRTV:** **Basis:** PPRTV is a tier 2 source, no tier 1 available. PPRTV (2009) p-RfC = 1.0E-4 mg/m^3: **Critical Study(ies)**: Gushow, T.S., R.R. Miller and B.L. Yano. 1984. Dowanol DB: A 5-week repeated vapor inhalation study in rats. Dow Chemical USA, Midland, MI. Submitted to U.S. EPA under TSCA Section 4, Fiche No. OTS0512379. (unpublished) **Method(s)**: F344 rats (15/sex/dose group) were exposed to 0, 2, 6, or 18 ppm of DGBE (0, 13, 40, or 119 mg/m^3) for 6 hours/day, 5 days/week, for up to 22 exposures in 5 weeks (average daily concentration: 0, 2.3, 7.1, or 21.3 mg/m^3). **Critical effect**: hepatic changes (hepatocelluar vacuolization) in female rats **End point or Point of Departure (POD):** $BMCL_{10HEC}$ = 0.32 mg/m^3 **Uncertainty Factors**: UF = 3,000 (10 each for interspecies variability, use of a sub chronic study and database deficiencies, and 3 for interspecies extrapolation (pharmacodynamics))		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Source and date: PPRTV, 9/28/2009 **Tier 1 and 2 Sources**: **IRIS:** No IRIS file available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, ITSL = 2.0E+1 µg/m³. See Part 201 Value RfC details.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: "there is inadequate information to assess the carcinogenic potential" **IRIS WOE Basis**: No adequate information on the carcinogenicity of DGBE due to a lack of oral, inhalation, or dermal studies in animals longer than 13 weeks in duration. Genotoxicity testing of DGBE in vitro with bacteria and mammalian cells and in vivo with Drosophila and mice have yielded negative results in all but one study. **Source and Date**: PPRTV, 9/28/2009 **Tier 1 and 2 Sources**: **IRIS:** No IRIS file available at this time. **PPRTV**: Per PPRTV (9/28/2009), no value 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	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, 2015	
SMCL details	NA	SDWA, 1976 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 (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)	NA	MDEQ, 2015
Target Detection Limit – Water (μg/L)	NA	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