CHEMICAL UPDATE WORKSHEET

Chemical Name:	**Ethyl acetate**
CAS #:	**141-78-6**
Revised By:	RRD Toxicology Unit
Revision Date:	July 31, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	88.12	88.11	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	190	-83.60	EPI	EXP
Boiling Point (˚C)	77.1	77.10	EPI	EXP
Solubility (ug/L)	6.40E+7	8.0000E+07	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	9.12	9.32E+01	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	1.70E-4	1.34E-04	EPI	EXP
Log Kow (log P; octanol-water)	0.69	0.73	EPI	EXP
Koc (organic carbon; L/Kg)	4.77	5.583	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.73	8.23E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	9.7E-6	9.70E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	24 F	-4	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.02	0.02	CRC	EXP
Critical Temperature (K)		523.30	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		7.63E+03	EPA2004	EXP
Density (g/mL, g/cm^3)		0.9003	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	2.41E-05	2.62E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	4.90E-05	5.71E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	3.36E-05	4.09E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	6.51E-05	8.59E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	9.0E-1	7.2E-2	PPRTV, 2013/MDEQ, 2015	
RfD details	Rat sub chronic gavage study (US EPA, 1986). NOAEL = 900 mg/kg/day; UF = 1000; Critical effects = mortality and body weight loss. Source: IRIS CCD Date: 6/11/1986	**Tier 2 Source:** **PPRTV:** **Basis:** The PPRTV subchronic p-RfD of 7.2E-1 mg/kg-day is used as it represents the most recent assessment. MDEQ applied an additional UF of 10 to account for subchronic to chronic exposure: chronic RfD = 7.2E-1 mg/kg-day. **PPRTV, 5/6/2013 Sub chronic p-RfD derivation:** **Critical Study**: American Biogenics Corporation. (1986) Rat oral sub chronic study with ethyl acetate. Office of Solid Waste, U.S. Environmental Protection Agency, Washington, DC. 699273. (unpublished) **Method(s)**: Sprague-Dawley rats (30/sex/group were exposed to 0, 300, 900, or 3600 mg/kg-day by daily gavage for up to 93 days. An interim sacrifice of 10 rats/sex/group was performed on Days 44−45; the remaining rats were sacrificed on Days 91−93. **Critical effect**: clinical signs, including increased salivation, irregular breathing, and lethargy in both sexes **End point or Point of Departure (POD):** NOAEL = 900 mg/kg-day; $NOAEL_{HED}$ = 216 mg/kg-day (derived by applying a dosimetric adjustment factor = 0.24 assuming BWa = 0.25 kg for rats and BWh = 70 kg for humans) **Uncertainty Factors**: UF = 300 (10 each for interspecies variability and database deficiencies, and 3 for interspecies extrapolation) **Tier 1 and 2 Sources:** **IRIS:** Per IRIS (3/01/1988), RfD = 9.0E-1 mg/kg-day. **Critical Study:** U.S. EPA. 1986. Rat oral sub chronic study with ethyl acetate. Office of Solid Waste, Washington, DC. (Also American Biogenics Corporation. (1986) Rat oral sub chronic study with ethyl acetate. Office of Solid Waste, U.S. Environmental Protection Agency, Washington, DC. 699273.) **Method(s):** Rats (30/sex/group) were exposed to 0, 300, 900 and 3600 mg/kg/day of ethyl acetate daily by gavage. Six weeks after the initial dosing, 10 rats/sex		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		were sacrificed. The remaining rats were dosed until the final sacrifice (90 days). **Critical effect:** mortality and body weight loss **End point or Point of Departure (POD):** NOEL = 900 mg/kg-day **Uncertainty Factors:** UF = 1,000 (10 each for interspecies variability, interspecies extrapolation and use of a sub chronic study) **Source and date:** IRIS, last revision date - 3/01/1988. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD (6/11/1988), RRD adopted IRIS RfD. See Part 201 Value RfD details.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	
CSF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: "Inadequate Information to Assess Carcinogenic Potential" **IRIS WOE Basis**: no adequate information available to assess carcinogenic potential. **Source and Date**: PPRTV, 5/6/2013 **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (3/01/1988), no value at this time. **PPRTV:** Per PPRTV (5/6/2013), 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
Reference Concentration (RfC) or Initial Threshold Screening Level	3.2E+3	7.0E+1	PPRTV, 2013	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(ITSL) (µg/m³)				
RfC/ITSL details	ITSL is based on conversion from EPA's RfD. The RfD is based on a NOAL of 900 mg/kg from 90 d, male rat gavage study which found decreased body weight and altered liver weights EPA (1986). FINAL. CCD/AQD date: 7/1/1992.	**Tier 2 Source:** **PPRTV:** **Basis:** PPRTV is a Tier 2 source, no Tier 1 available. PPRTV chronic p-RfC = 7.0E-2 mg/m^3: **Critical Study**: Christoph, GR; Hansen, JF; Leung, HW. (2003) Sub chronic inhalation neurotoxicity studies of ethyl acetate in rats. Neurotoxicology 24(6):861−874. **Method(s)**: Sprague-Dawley rats were exposed to 0 (n = 18/sex), 350 (n = 12/sex), 750 (n = 12/sex), or 1500 (n = 18/sex) ppm ethyl acetate by whole-body inhalation for 6 hours/day, 5 days/week for 13 weeks. The exposure was interrupted for neurobehavioral testing; however, each rat received a total of 65 exposures. Adjustment based on 65 doses resulted in the following HEC estimates: 0, 209, 448, and 896 mg/m^3. **Critical effect**: decreased body weights, body-weight gains, food efficiency, and startle response in both sexes and decreased food consumption in males. **End point or Point of Departure (POD):** $NOAEL_{HEC}$ = 209 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) **Source and date:** PPRTV, 5/6/2013 **Tier 1 and 2 Sources:** **IRIS:** Per IRIS (8/01/1989), no value at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD/AQD (7/1/1992), RfC = 3.2E+3 µg/m³. See Part 201 Value RfC details.		Complete
Inhalation Unit Risk Factor (IURF) ($(µg/m^3)^{-1}$)	--	NA	MDEQ, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
IURF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: "Inadequate Information to Assess Carcinogenic Potential" **IRIS WOE Basis**: no adequate information available to assess carcinogenic potential. **Source and Date**: PPRTV, 5/6/2013 **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (3/01/1988), no value at this time. **PPRTV:** Per PPRTV (5/6/2013), 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.		
Developmental or Reproductive Effector? (Y/N)	No	No. The RfD and ITSL are 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	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	8.80E+02	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	2.90E+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