



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Acetaldehyde</b>
<b>CAS #:</b>	<b>75-07-0</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	November 16, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	44.1	44.05	EPI	EXP
<b>Physical State at ambient temp</b>	Liquid	Gas	MDEQ	
<b>Melting Point (°C)</b>	---	-123.37	EPI	EXP
<b>Boiling Point (°C)</b>	20.1	20.10	EPI	EXP
<b>Solubility (ug/L)</b>	1.0E+9	1.00E+09	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	740	9.02E+02	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	7.95E-5	6.67E-05	EPI	EXP
<b>Log Kow (log P; octanol-water)</b>	-0.367	-0.34	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	0.613	1	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	1.28E-01	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	1.353E-05	W9	EST
<b>Soil Water Partition Coefficient (Kd; inorganics)</b>	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	-36	-39	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.04	0.04	CRC	EXP
Critical Temperature (K)		466.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		6.16E+03	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.7834	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.35E-05	2.60E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	4.55E-05	5.63E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	3.26E-05	4.06E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	5.97E-05	8.44E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.3E-1	1.3E-1	MDEQ, 1993	
RfD details	4-week drinking-water study in rats. NOAEL=125 mg/kg. Critical Effect = hyperkeratoses of the forestomach, UF=1000. CCD/RRD date: 12/20/1993	<p><b>Tier 3 Source:</b>  <b>MDEQ:</b>  <b>Basis:</b> The MDEQ (1993) value is used based on a NOAEL of 125 mg/kg-day. The Texas value used the same critical study and UF value; however, the Texas justification reports two different NOAELs and the NOAEL of 102 mg/kg-day was used to derive the RfD with no explanation provided. For this reason, the DEQ value was used. See details below.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (6/30/88), no value at this time  <b>PPRTV:</b> No PPRTV record is available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b> Per MDEQ-CCD/RRD (12/20/1993), RfD = 1.3E-1 mg/kg-day  <b>Critical Study:</b> Til HP, Woutersen RA, Feron VJ, Clary JJ (1988). Evaluation of the oral toxicity of acetaldehyde and formaldehyde in a 4-week drinking water study in rats. Food Chem Toxicol. 26(5):447-52.(ecopy in tox assessment folder)  <b>Method(s):</b> 4-week drinking water study; five week old rats (10/dose/sex and 20/sex for control animals) dosed at 0, 25, 125, or 675 mg/kg/day  <b>Critical effect:</b> hyperkeratosis of the forestomach.  <b>End point or Point of Departure (POD):</b> NOAEL = 125 mg/kg/day  <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability and interspecies and subchronic-to-chronic extrapolation).  <b>Source and date:</b> MDEQ-ERD, 12/20/1993</p> <p><b>Texas CEQ:</b> RfD= 1.0E-01 mg/kg/day.  Justification:  <b>Key study:</b> Evaluation of the oral toxicity of acetaldehyde and formaldehyde in a</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>4-week drinking-water study in rats. Til HP, Woutersen RA, Feron VJ, Clary JJ. Food Chem Toxicol 1988 May; 26(5):447-52.</p> <p>Methods: A subacute oral toxicity study of acetaldehyde and formaldehyde was carried out in rats. Groups of ten male and ten female 5-wk-old rats received one of the aldehydes in the drinking-water for a period of 4 wk., acetaldehyde being given at dose levels of 25, 125 and 675 mg/kg body weight/day and formaldehyde at dose levels of 5, 25 and 125 mg/kg body weight/day. A group of 20 males and 20 females served as controls and received unsupplemented drinking-water ad lib. An additional group of ten males and ten females was given unsupplemented drinking-water in an amount equal to the amount of liquid consumed by the group given the top dose of formaldehyde. Food and liquid intake were decreased in the groups on the top dose of both acetaldehyde and formaldehyde.</p> <p>Hyperkeratosis of the forestomach, observed only in the top-dose rats, was the only adverse effect of acetaldehyde detected. Effects of formaldehyde, also observed only in the top-dose group, were yellow discoloration of the fur, decreased protein and albumin levels in the blood plasma, thickening of the limiting ridge and hyperkeratosis in the forestomach, and focal gastritis in the glandular stomach. It was concluded that in this study the NOAELs for acetaldehyde and formaldehyde were 125 and 25 mg/kg body weight/day, respectively.</p> <p><b>NOAEL</b> = 102 mg/kg-day (the NOAEL is reported as two different numbers in the TX justification.</p> <p><b>Uncertainty Factors:</b> 1,000 (10 each for Interspecies Extrapolation, Interspecies Extrapolation, and Use of Subacute Study)</p> <p><b>Source:</b> TCEQ Communication, 3/15/2001</p> <p><b>Other Tier 3:</b> 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), ECHA (REACH) and OECD HPV.</p>		
<b>Oral Cancer Slope Factor (CSF)</b>	--	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
(mg/kg-day) <sup>-1</sup> )				
CSF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> B2 - probable human carcinogen  <b>IRIS WOE Basis:</b> Based on increased incidence of nasal tumors in male and female rats and laryngeal tumors in male and female hamsters after inhalation exposure  <b>Source and Date:</b> IRIS, 1/1/1991</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (1/1/1991), no value is available at this time.  <b>PPRTV:</b> No PPRTV record is available at this time.  <b>MRL:</b> NA; MRLs are for non-cancer health effects only.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m <sup>3</sup> )	9.0E+0	9.0E+0	IRIS, 1991	
RfC/ITSL details	ITSL was based on EPA RfC from Appleman et al 1986, 4 week rat inhalation study. CCD/AQD date: 4/25/1991	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is the only available value.  <b>Critical Studies:</b> Appleman et al.,1986;1982                      1) Appleman, L.M., R.A. Woutersen, V.J. Feron, R.N. Hooftman and W.R.F. Notten. 1986. Effect of variable versus fixed exposure levels on the toxicity of acetaldehyde in rats. J. Appl. Toxicol. 6(5): 331-336; and                      2) Appleman, L.M., R.A. Woutersen, and V.J. Feron. 1982. Inhalation toxicity of acetaldehyde in rats. I. Acute and subacute studies. Toxicology. 23: 293-297  <b>Method(s):</b> two inhalation studies on male Wistar rats exposed 6 hours/day, 5 days/week for 4 weeks to 0, 150, and 500 ppm (0, 273 and 910 mg/ m<sup>3</sup>, respectively). Duration-adjusted concentrations are 0, 48.75, and 162.5 mg/ m<sup>3</sup>, respectively 4-week exposure.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Critical effect:</b> degeneration of olfactory epithelium in the extra thoracic region  <b>End point or Point of Departure (POD):</b> NOAEL = 150 ppm (257 mg/ m<sup>3</sup>); NOAEL<sub>HEC</sub> = 8.7 mg/ m<sup>3</sup> (from Appleton et al 1986)  <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability use of subchronic study and, interspecies extrapolation /database insufficiency).  <b>Source and date:</b> IRIS, Last revision date - 10/01/1991</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> No PPRTV record is available at this time  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD (4/25/91), AQD adopted IRIS RfC.</p>		
<b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b>	2.2E-6	2.2E-6	IRIS, 1991	
<b>IURF details</b>	<p>Potency from IRIS is based on increased incidence of male rat nasal squamous cell carcinoma or adenomas following inhalation exposure reported by Woutersen &amp; Appelman 1984. CCD/AQD date: 4/25/1991</p>	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is the only available value.  <b>Critical Study:</b> Woutersen, R.A. and L.M. Appelman (1984). Lifespan inhalation carcinogenicity study of acetaldehyde in rats. III. Recovery after 52 weeks of exposure. Report No. V84.288/190172. CIVO-Institutes TNO, The Netherlands.  <b>Method(s):</b></p> <ol style="list-style-type: none"> <li>1) Dose response data: Tumor Type - nasal squamous cell carcinoma or adenocarcinoma; Test Species - rat/SPF Wistar, male; Route - inhalation</li> <li>2) Extrapolation method: Linearized multistage-variable exposure input form (extra risk)</li> </ol> <p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> B2; probable human carcinogen  <b>IRIS WOE Basis:</b> increased incidence of nasal tumors in male and female rats and laryngeal tumors in male and female hamsters after inhalation exposure  <b>Source and Date:</b> IRIS; Last revision date - 01/01/1991</p> <p><b>Tier 2 Sources:</b></p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<b>PPRTV:</b> No PPRTV record is available at this time. <b>MRL:</b> ATSDR MRLs are for non-cancer health effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD (4/25/91), AQD adopted IRIS IUR.		
<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>	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<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		
<b>Secondary Maximum Contaminant Level (SMCL) (ug/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List		
<b>Is there an Aesthetic Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Aesthetic value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Others				

**(C) Chemical-specific Absorption Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
<b>Gastrointestinal absorption efficiency value (ABS<sub>gi</sub>)</b>	---	1.0	MDEQ, 2015/USEPA RAGS-E	
<b>ABS<sub>gi</sub> details</b>		RAGS E (EPA, 2004) Default Value		
<b>Skin absorption efficiency value (AE<sub>d</sub>)</b>	---	0.1	MDEQ, 2015	
<b>AE<sub>d</sub> details</b>				
<b>Ingestion Absorption Efficiency (AE<sub>i</sub>)</b>		1.0	MDEQ, 2015	
<b>AE<sub>i</sub> Details</b>				
<b>Relative Source Contribution for Water (RSC<sub>w</sub>)</b>		0.2	MDEQ, 2015	
<b>Relative Source Contribution for Soil (RSC<sub>s</sub>)</b>		1.0	MDEQ, 2015	
<b>Relative Source Contribution for Air (RSC<sub>a</sub>)</b>		1.0	MDEQ, 2015	
<b>Others</b>				

**(D) Rule 57 Water Quality Values and GSI Criteria**

<b>Current GSI value (µg/L)</b>	130
<b>Updated GSI value (µg/L)</b>	130
<b>Rule 57 Drinking Water Value (µg/L)</b>	1,200

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	1,200	7/2001
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	93,000	7/2001
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	NA	NA
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	NA	NA
<b>Final Chronic Value (FCV)</b>	130	7/2001
<b>Aquatic maximum value (AMV)</b>	1,200	7/2001
<b>Final Acute Value (FAV)</b>	2,400	7/2001

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)

**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	2,500	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	100	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	4.90E+00	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	1.60E+02	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