



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Acrolein
CAS #:	107-02-8
Revised By:	RRD Toxicology Unit
Revision Date:	August 12 , 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	56.06	56.06	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	185	-87.70	EPI	EXP
Boiling Point (°C)	52.6	52.60	EPI	EXP
Solubility (ug/L)	2.10E+8	2.12E+08	EPI	EXP
Vapor Pressure (mmHg at 25°C)	266	2.74E+02	EPI	EXP
HLC (atm-m³/mol at 25°C)	9.40E-5	1.22E-04	EPI	EXP
Log Kow (log P; octanol-water)	-0.01	-0.01	EPI	EXP
Koc (organic carbon; L/Kg)	1.18	1	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.11	1.12E-01	W9	EST
Diffusivity in Water (Dw; cm²/s)	1.2E-5	1.2208E-05	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	-15 F	-26	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.028	0.028	CRC	EXP
Critical Temperature (K)		506.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		6.73E+03	EPA2004	EXP
Density (g/mL, g/cm ³)		0.84	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	2.43E-05	2.66E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	4.96E-05	5.98E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	3.38E-05	4.18E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	6.63E-05	9.12E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	1.6E-2	4.0E-3	ATSDR, 2007	
RfD details	Subchronic (90-day) drinking water study in rats (EPA, 1985) NOAEL = 15.6 mg/kg; UF = 1000. SWQ developed RFD of 1.2E-4 mg/kg/day. CCD/WRD date:	<p>Tier 2 Source: Basis: ATSDR intermediate oral MRL = 0.004 or 4.0E-3 mg/kg/day. A chronic oral MRL is not available at this time. ATSDR is more recent than IRIS. ATSDR: Critical Study: NTP. 2006. NTP technical report on the comparative toxicity studies of allyl acetate, allyl alcohol, and acrolein administered by gavage to F344/N rats and B6C3F1 mice (Tox report #48). National Toxicology Program. Method(s): Groups of 10 rats/sex/dose were exposed to 0.75, 1.25, 2.5, 5, and 10 mg/kg/day by gavage for 14 weeks, while groups of 10 mice/sex/dose were given 1.25, 2.5, 5, 10, and 20 mg/kg for the same duration. Dose volumes were 5 mL/kg for rats and 10 mL/kg for mice. Critical effect: forestomach squamous epithelial hyperplasia in mice End point or Point of Departure (POD): BMDL₁₀ = 0.36 mg/kg/day. Uncertainty Factors: UF = 100 (10 each for interspecies extrapolation and intraspecies variability) Source and date: ATSDR, 08/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (6/03/2003), RfD = 5.0E-4 mg/kg-day. Critical Study: Parent, RA; Caravello, HE; Long, JE. (1992) Two-year toxicity and carcinogenicity study of acrolein in rats. J Appl Toxicol 12(2):131-139. Method(s): Sprague Dawley rats (70/dose/sex) were exposed to 0, 0.05, 0.5, or 2.5 mg/kg/day via daily oral gavage in water for up to two years. Critical effect: decreased survival of both male and female rats End point or Point of Departure (POD): NOAEL = 0.05 mg/kg/day. Uncertainty Factors: UF = 100 (10 each for interspecies extrapolation and intraspecies variability) Source and date: IRIS, Last revision date - 6/03/2003; An IRIS Toxicology Review is available.</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>PPRTV: Per PPRTV (4/30/2002), no value at this time.</p> <p>Tier 3 Source: MDEQ: Per CCD/WRD, RfD = 1.6E-2 mg/kg-day. See Part 201 Value RfD details.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ,2015	
CSF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: "data are inadequate for an assessment of human carcinogenic potential for either the oral or inhalation route of exposure." WOE Basis: Per IRIS (2003), the highly reactive nature of acrolein and studies supporting the lack of systemic distribution of acrolein suggest that acrolein is not likely to reach potential target sites at a sufficient concentration to initiate a carcinogenic process in mammalian species. Per EPA-OPP (8/2009), "the potential carcinogenicity of acrolein is inconclusive; however, exposure to parent acrolein is not expected. Glycidol is a metabolite of acrolein in fish. Glycidol is anticipated to be a human carcinogen by NTP and IARC. To quantify the carcinogenic response of glycidol, a multistage model BMD analysis was performed to derive a cancer slope factor of 0.16 mg-1kg-1day-1 at a 0.95 confidence level." Source and date: IRIS, 6/03/2003; OPP, 8/2009</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (06/03/03), no value at this time. PPRTV: Per PPRTV (4/30/2002), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per MDEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level	2.0E-2	2.0E-2	IRIS, 2003	

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
(ITSL) (µg/m³)				
RfC/ITSL details	Based on EPA's RfC from Kutzman 1981 62 day rat inhalation study and supported by Feron et al 1978.	<p>Tier 1 Source: IRIS: Per IRIS (6/06/2003), RfC = 2.0E-2 µg/m³. IRIS is a Tier 1 source. Critical Study: Feron, VJ; Kryusse, A; Til, HP; et al. (1978) Repeated exposure to acrolein vapor: subacute studies in hamsters, rats and rabbits. Toxicology 9:47-57. Method(s): Wistar rats (6/sex/concentration), Syrian golden hamsters (10/sex/concentration), and Dutch rabbits (2/sex/concentration) were exposed for 6 hr/day, 5 days/week for 13 weeks to 0, 0.4, 1.4, or 4.9 ppm (0, 0.9, 3.2, or 11 mg/m³) in a whole-body exposure chamber Critical effect: nasal lesions End point or Point of Departure (POD): LOAEL = 0.4 ppm (0.9 mg/m³), LOAEL (ADJ) = 0.16 mg/m³, LOAEL (HEC) = 0.02 mg/m³ Uncertainty Factors: UF = 1,000 (10 each for intra-species variability, interspecies, and sub-chronic to chronic extrapolation, and 3 for use of a LOAEL). Source and date: IRIS, Last revision date - 06/03/2003</p> <p>Other Sources: PPRTV: Per PPRTV (4/302002), no value at this time. MRL: Per ATSDR (8/2007), no chronic inhalation MRL at this time. An intermediate inhalation MRL = 0.00004 or 4.0E-5 ppm is derived as follows: Critical Study: Feron, VJ; Kryusse, A; Til, HP; et al. (1978) Repeated exposure to acrolein vapor: subacute studies in hamsters, rats and rabbits. Toxicology 9:47-58. Method(s): Wistar rats (6/sex/group), Syrian golden hamsters (10/sex/group), and Dutch rabbits (2/sex/group) were exposed to 0, 0.4, 1.4, or 4.9 ppm (0, 0.9, 3.2, or 11 mg/m³) in a whole-body exposure chamber for 6 hours/day, 5 days/week for 13 weeks. Critical effect: nasal epithelial metaplasia End point or Point of Departure (POD): LOAEL = 0.4 ppm (0.9 mg/m³), LOAEL (ADJ) = 0.071 ppm (0.16 mg/m³); LOAEL (HEC) = 0.012 ppm (0.02 mg/m³) Uncertainty Factors: UF = 1,000; A UFA of 3 (101/2) was used for interspecies extrapolation, since this factor embodies two areas of uncertainty: pharmacokinetics and pharmacodynamics. In this assessment, the</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>pharmacokinetic component was addressed by the calculation of the human equivalent concentration (HEC) according to the procedures in the RfC methodology (U.S. EPA, 1994b). Accordingly, only the pharmacodynamic area of uncertainty remains as a partial factor for interspecies uncertainty (10^{1/2} or approximately 3). A default UFH of 10 was applied for interspecies uncertainty to account for human variability and sensitive subpopulations, i.e., to account for human variability in the severity or range of response from any given acrolein exposure amongst different individuals. A UFS of 10 was applied for adjustment from sub chronic to chronic duration because the principal study involved a 13-week dosing period and because there are insufficient inhalations data to preclude an increase in severity (or incidence) with an increase in exposure duration from sub chronic to chronic. A UFL of 3 (10^{1/2}) was applied for use of a minimal LOAEL of 0.4 ppm (0.9 mg/m³) in lieu of a NOAEL. Although the severity of the nasal effect at the 0.4 ppm level was minimal and in only 1 of 12 animals in the Feron et al. (1978) study, a 3-day study in the male Wistar rat by Cassee et al. (1996) also reported slight nasal effects in the respiratory/transitional epithelium from nose-only inhalation exposure at 0.25 ppm (0.6 mg/m³). An exposure concentration of 0.4 ppm (0.9 mg/m³) was designated a minimal LOAEL instead of a NOAEL, considering the Cassee et al. (1996) results and the observed increase in the severity of the effects with increasing dose in the Feron et al. (1978) study.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD (6/14/2013), ITSL = 0.16 µg/m³. IRIS value was adjusted using a DAF of 1 in place of 0.14.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m³)⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: "data are inadequate for an assessment of human carcinogenic potential for either the oral or inhalation route of exposure." WOE Basis: Per IRIS (2003), the highly reactive nature of acrolein and studies supporting the lack of systemic distribution of acrolein suggest that acrolein is not likely to reach potential target sites at a sufficient concentration to initiate a</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>carcinogenic process in mammalian species. Per EPA-OPP (8/2009), “the potential carcinogenicity of acrolein is inconclusive; however, exposure to parent acrolein is not expected. Glycidol is a metabolite of acrolein in fish. Glycidol is anticipated to be a human carcinogen by NTP and IARC. To quantify the carcinogenic response of glycidol, a multistage model BMD analysis was performed to derive a cancer slope factor of 0.16 mg-1kg-1day-1 at a 0.95 confidence level.”</p> <p>Source and date: IRIS, 6/03/2003; OPP, 8/2009</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (06/03/03), no value at this time. PPRTV: Per PPRTV (4/30/2002), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per MDEQ-CCD, no value at this time.</p>		
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	--	NO	SDWA, 1976 and USEPA SMCL List	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(SMCL) (ug/L)				
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 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	
ABS _{gi} details				
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 ($\mu\text{g}/\text{kg}$)	250	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	20	MDEQ, 2015
Target Detection Limit – Air (ppbv)	8.60E-03	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	2.90E-01	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