CHEMICAL UPDATE WORKSHEET

Chemical Name:	**Acrylonitrile**
CAS #:	**107-13-1**
Revised By:	RRD Toxicology Unit
Revision Date:	November 16, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	53.06	53.06	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (˚C)	191	-83.50	EPI	EXP
Boiling Point (˚C)	77.3	77.30	EPI	EXP
Solubility (ug/L)	7.50E+7	7.45E+07	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	106.4	1.09E+02	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	1.00E-4	1.38E-04	EPI	EXP
Log Kow (log P; octanol-water)	0.255	0.25	EPI	EXP
Koc (organic carbon; L/Kg)	1.78	8.511	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.12	1.14E-01	W9	EST
Diffusivity in Water (Dw; cm^2/s)	1.3E-5	1.226E-05	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	30 F	0	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.03	0.03	CRC	EXP
Critical Temperature (K)		519.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		7.79E+03	EPA2004	EXP
Density (g/mL, g/cm^3)		0.8007	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	2.44E-05	2.64E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	5.01E-05	5.86E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	3.40E-05	4.14E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	6.71E-05	8.87E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	--	1.0E-2	ATSDR, 1990	
RfD details	NA	**Tier 2 Source:** **ATSDR:** **Basis:** ATSDR critical study is more current than that used by IRIS and MDEQ. The oral intermediate MRL = 0.01 mg/kg-day is based on reproductive effects: **Critical Study**: Tandon R, Saxena DK, Chandra SV, et al. 1988. Testicular effects of acrylonitrile in mice. Toxicol Lett 42:55-63. **Method(s)**: Mice were exposed to 10 mg/kg-day by gavage daily for 60 days **Critical effect:** reduced sperm count and degeneration of testicular tubules **End point or Point of Departure (POD):** LOAEL = 10 mg/kg-day) **Uncertainty Factors**: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation, and use of a LOAEL) **Source and date:** ATSDR, 12/1990. Toxicological Profile is available **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (7/01/1993), no value at this time. **PPRTV:** No PPRTV record available at this time **MRL:** ATSDR (12/1990) derived an oral **chronic** MRL = 0.04 mg/kg/day. From 12/2014 MRL List. **Critical Study**: Bio/dynamics. 1980b. A twenty-four month oral toxicity/carcinogenicity study of acrylonitrile administered in the drinking water to Fischer 344 rats. Biodynamics, Inc., Division of Biology and Safety Evaluation, East Millstone, NJ. Project No. BDN-77-27. (unpublished) **Method(s)**: 24-month drinking water study in F344 rats exposed to 10, 14, or 25 mg/kg-day (verify doses) **Critical effect:** decreased red cells **End point or Point of Departure (POD):** NOAEL = 4.2 mg/kg-day **Uncertainty Factors**: UF = 100 (10 each for intraspecies variability and interspecies extrapolation)		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		ATSDR also derived an acute oral MRL = 0.1 ppm based on developmental effects. **Critical Study**: Murray FJ, Schwetz BA, Nitschke KD, et al. 1978. Teratogenicity of acrylonitrile given to rats by gavage or by inhalation. Food Cosmet Toxicol 16:547-551. **Method(s)**: Rats were exposed by to 10, 25 or 65 mg/kg-day for 6 hrs./day during gestation (GD 6-15) **Critical effect:** malformations **End point or Point of Departure (POD):** NOAEL = 10 mg/kg-day) **Uncertainty Factors**: UF = 1,000 **Tier 3 Source:** **MDEQ:** Per MDEQ/WRD (8/17/2007), RfD = 2.5E-3 mg/kg-day **Critical Study (ies)**: Bio/dynamics. 1980b. A twenty-four month oral toxicity/carcinogenicity study of acrylonitrile administered in the drinking water to Fischer 344 rats. Biodynamics, Inc., Division of Biology and Safety Evaluation, East Millstone, NJ. Project No. BDN-77-27. (unpublished) **Method(s)**: 24-month drinking water study in F344 rats **Critical effect:** cancer and noncancerous effects **End point or Point of Departure (POD):** NOAEL = 3 ppm (0.25 mg/kg/d) **Uncertainty Factors**: UF = 100 (10 each for intraspecies variability and interspecies extrapolation) **Source and date:** MDEQ-WRD, 8/17/2007		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	3.3E-1	5.4E-1	IRIS, 1991	
CSF details	Increase in brain astrocytomas in female Sprague-Dawley rats exposed via the drinking water for 2 years (Quast, 1980). Revised	**Tier 1 Source:** **IRIS:** **Basis:** Per IRIS (1/1/1991), CSF = 5.4E-1 (mg/kg-day)$^{-1}$. IRIS selected because it is a Tier 1 source. **Critical Studies:** Biodynamics (1980a), Biodynamics (1980b), and Quast et al. (1980) **Method(s):** The CSF is a geometric mean (5.4E-1 per mg/kg/day) of these three slope factors: 4.0E-1 (Biodynamics, 1980a), 4.0E-1 (Biodynamics, 1980b) and 9.9E-		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	species scaling factor of (BWh/BWa) to the 0.25 power used for q* calculation.	1 per (mg/kg)/day (Quast et al., 1980). The overall risk of tumors was determined from the number of animals having tumors that were statistically significant at any site. Tumors (brain and spinal cord astrocytomas, Zymbal gland carcinomas and stomach papilloma/carcinomas) were observed in studies in two rat strains (Sprague Dawley and F344) exposed by various routes (drinking water, gavage, and inhalation). Extrapolation Method — Linearized multistage procedure, extra risk **Carcinogen Weight-of-Evidence (WOE) Class:** B1; probable human carcinogen **IRIS WOE Basis:** statistically significant increase in incidence of lung cancer in exposed workers and observation of tumors, generally astrocytomas in the brain, in studies in two rat strains exposed by various routes (drinking water, gavage, and inhalation). **Source and Date:** IRIS, Last revision date – 1/1/1991 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** Per MDEQ/WRD, CSF = 1.4E+0 $(mg/kg\text{-}day)^{-1}$ **Critical Study**: Ghanayem et al. (2002). **Methods**: Male and female B6C3F1 mice were gavaged 5 days per week for 2 years. SAD = 0, 1.79, 7.14, or 14.29 mg/kg/day. The incidences for combined forestomach papilloma and carcinomas and Harderian gland adenomas increased in both sexes. Male data were used because they resulted in the highest slope factor. **Source and Date** MDEQ/WRD, 8/17/2007.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	2.0E+0	2.0E+0	IRIS, 1991	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
RfC/ITSL details	Based on EPA's RfC from Quast et al 1980, 2 year rat inhalation study effects on nasal epithelium.	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. **Critical Studies**: Quast J.F., D.J. Schwetz, M.F. Balmer, T.S. Gushow, C.N. Park and M.J. McKenna. 1980. A two-year toxicity and oncogenicity study with acrylonitrile following inhalation exposure of rats. Dow Chemical Co., Toxicology Research Laboratory, Midland, MI **Methods**: Sprague-Dawley rats (100/sex/concentration) were exposed to 0, 20 or 80 ppm acrylonitrile (duration-adjusted concentrations of 7.7 and 31 mg/m3) 6 hours/day, 5 days/week for 2 years The control group was exposed only to air. **Critical effect**: Degeneration and inflammation of nasal respiratory epithelium; hyperplasia of mucous secreting cells **End point or Point of Departure (POD):** LOAEL = 43 mg/m3 (20 ppm), LOAEL (ADJ) = 7.7 mg/m3, LOAEL (HEC) = 1.9 mg/m3 **Uncertainty Factors**: UF = 1,000 (10 each for intra-species variability and incomplete database, and 3 each for interspecies and LOAEL to NOAEL extrapolation) **Source and date:** IRIS, Last revision date – 12/01/1991 **Tier 2 Sources:** **PPRTV:** No PPRTV record available at this time **MRL:** Per ATSDR (12/1990), no chronic inhalation MRL at this time. ATSDR derived an acute inhalation MRL = 0.1 ppm based on developmental effects. **Critical Study**: Jakubowski M, Linhart I, Pielas G, et al. 1987. 2-Cyanoethylmer-capturic acid (CEMA) in the urine as a possible indicator of exposure to acrylonitrile. Br J Ind Med 44:834-840. **Methods**: human exposure for 8 hours. Dose adjusted for intermittent exposure **Critical effect:** neurological **End point or Point of Departure (POD):** NOAEL = 4.6 ppm **Uncertainty Factors**: UF = 10 (intraspecies variability) **Source and date:** ATSDR, 12/1990		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Tier 3 Source: **MDEQ:** Per DEQ-CCD (date), AQD adopted the IRIS value.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	6.8E-5	6.8E-5	IRIS, 1991	
IURF details	Potency is based on EPA's IRIS value as calculated from OBerg et al 1980.	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is the only available value. **Critical Study**: O'Berg, M. 1980. Epidemiologic study of workers exposed to acrylonitrile. J. Occup. Med. 22: 245-252. **Method(s)**: 1) *Dose response data*: *Tumor Type* - respiratory cancer; *Test Species* - humans; *Route* - inhalation 2) *Extrapolation method*: The unit risk was calculated from a relative risk model adjusted for smoking and based on a continuous lifetime equivalent of occupational exposure. **Carcinogen Weight-of-Evidence (WOE) Class**: B1; probable human carcinogen **IRIS WOE Basis**: statistically significant increase in incidence of lung cancer in exposed workers and observation of tumors, generally astrocytomas in the brain, in studies in two rat strains exposed by various routes (drinking water, gavage, and inhalation). **Source and Date**: IRIS, Last revision date – 1/01/1991 **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** NA; MRLs are for non-cancer effects only. **Tier 3 Source:** **MDEQ:** AQD adopted IRIS value for IURF. 2/11/1987		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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 nor RfC basis is not considered a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	**Critical effect:** reduced sperm count and degeneration of testicular tubules **Critical Study (ies)**: Tandon R, Saxena DK, Chandra SV, et al. 1988. Testicular effects of acrylonitrile in mice. Toxicol Lett 42:55-63. **Method(s)**: Mice were exposed to 10 mg/kg-day by gavage daily for 60 days		
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		
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	
ABSgi details		RAGS E (EPA, 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)	2.0 (M); 1.2
Updated GSI value (µg/L)	2 (M,X); 1.2
Rule 57 Drinking Water Value (µg/L)	2 (M); 0.21

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	58	8/2007
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	320	8/2007
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	0.21	8/2007
Human Cancer values for non-drinking water source (HCV-Non-drink)	1.2	8/2007
Final Chronic Value (FCV)	66	10/2010
Aquatic maximum value (AMV)	590	10/2010
Final Acute Value (FAV)	1,200	10/2010

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)	100	MDEQ, 2015
Target Detection Limit – Water (μg/L)	2	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.70E-01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	5.80E+00	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