CHEMICAL UPDATE WORKSHEET

Chemical Name:	**Caprolactam(DD)**
CAS #:	**105-60-2**
Revised By:	RRD Toxicology Unit
Revision Date:	September 16, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	113.2	113.16	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (˚C)	---	69.30	EPI	EXP
Boiling Point (˚C)	180	270.00	EPI	EXP
Solubility (ug/L)	5.25E+9	7.72E+08	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	0.0019	1.90E-03	HSDB	EXP
HLC (atm-m^3/mol at 25˚C)	2.53E-8	2.53E-08	PP	EST
Log Kow (log P; octanol-water)	-0.19	0.66	PP	EST
Koc (organic carbon; L/Kg)	0.65	24.5	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	6.89E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	8.9464E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	282 F	125	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.014	0.014	NPG	EXP
Critical Temperature (K)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		1.31E+04	HSDB	EXP
Density (g/mL, g/cm^3)		1.01	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	NA	1.34E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	NA	1.34E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	NA	1.68E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	NA	1.68E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	8.0E-1	5.0E-1	IRIS, 1988	
RfD details	Oral rat three generation reproductive studies. Critical effect = reduce offspring body weight. NOAEL=1000 ppm in diet = 83 mg/kg-d. UF=100; Serotta et al., 1984. 8.3% of body weight used as food consumed. *RfD Based on 8%BW Fd. Consmptn. TOC=59.7ppm(Vers.'83) CCD date: 9/1/1988	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is a Tier 1 source. **IRIS** RfD = 5.0E-1 mg/kg-day **Critical Study**: Serota, C.G., A.M. Hoberman and S.C. Gad. 1984. A three-generation reproduction study with caprolactam in rats. In: Proc. Symp. Ind. Approach Chem. Risk Assess: Caprolactam Relat. Compd. Case Study. Ind. Health Found. Pittsburgh, PA. p. 191-204 **Methods**: F344 rats (10 male and 20 female per dose) were administered 1000, 5000 or 10,000 ppm caprolactam in diets for three-generations. **Critical effect**: reduced offspring body weight **End point or Point of Departure (POD):** NOAEL = 1000 ppm (converted to 50 mg/kg/day). **Uncertainty Factors**: UF = 100 (10 each for intra-species variability and interspecies extrapolation). **Source and date:** IRIS, Last revision date - 9/07/88. An EPA screening-level review conducted in 2001 identified one or more significant new studies. **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per CCD/RRD (9/1/1988), RfD = 8.0E-1 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	**Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/07/88), no value at this time. Caprolactam has not undergone a		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		complete evaluation and determination for evidence of human carcinogenic potential. **PPRTV:** No PPRTV record available 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)	1.0E+1	2.2	CALEPA, 2013	
RfC/ITSL details	ITSL based on 1% of the NIOSH REL for both dust and vapor, per R232 (1) (c) (UF=100); critical effects are skin and respiratory irritation (Fed Regis 54(12):2454-2455). AQD, 5/26/1995	**Tier 3 Source:** **CALEPA:** **Basis:** California Chronic reference exposure level is based on a 2013 assessment of more current studies, including the key inhalation study. See details below. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/07/88), no value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Sources:** **MDEQ**: ITSL = 1.0E+1 µg/m³ **Basis**: MDEperoXisome1954Q-AQD ITSL is based on 1% of the NIOSH REL for both dust and vapor, per R232(1)(c) (UF=100) **Critical effect**: skin and respiratory irritation **Uncertainty Factors**: UF = 100 **Source and date:** MDEQ-AQD, 5/26/1995 **California (CALEPA):** Chronic reference exposure level (REL)= 2.2 µg/m^3. Study: Reinhold R.W. et al. 1988. Chronic Inhalation Toxicity Study of Caprolactam		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		(with a 4-Week Recovery) in the Rat via Whole-Body Exposures. Toxicological Sciences 44, 197-205. Study population: Sprague-Dawley CD rats (10 animals/sex/group) Exposure method: Discontinuous whole-body inhalation exposure to 0, 24, 70, and 243 mg/m^3 caprolactam aerosol Critical effects: Upper airway lesions of nasal and laryngeal epithelium LOAEL: 24 mg/m^3; NOAEL: Not observed BMCL05: 3 mg/m^3 Exposure continuity: 6 hours per day, 5 days/week Exposure duration: 13 weeks Average experimental exposure: 0.536 mg/m^3 (3 mg/m^3 x 6/24 hr. x 5/7 days) Human equivalent concentration: 0.134 mg/m^3 (for extra thoracic respiratory effects, RGDR = 0.25 Uncertainty factors (UF): 60; 2 for 13-wk exposure in rodents, 10 for toxicodynamic (UFA-d), and 10 for toxicodynamic (UFH-d) (potential asthma exacerbation in children) Source: OEHHA Reference Exposure Levels for Caprolactam, 2013 **Minnesota PCA:** RfC= 2.2 µg/m^3 based on California REL. Source: Minnesota Remediation Soil Remediation Value Spreadsheet - Draft, 2015 and Toxicity Values Used by MPCA for Air Toxics Comparisons. **ECHA (REACH):** Derived No Effect Level (DNEL) = 2.5 mg/m^3 (2.5E+3 µg/m^3). Overall assessment factor (AF) = 2. Most sensitive endpoint: irritation (respiratory tract) Overall assessment factor (AF): 2 Reference: Reinhold R.W. et al. 1988. Chronic Inhalation Toxicity Study of Caprolactam (with a 4-Week Recovery) in the Rat via Whole-Body Exposures. Toxicological Sciences 44, 197-205. Method: male and female Sprague-Dawley rats (10/sex/dose) were exposed to 0, 0.025, 0.075 and 0.250 mg/l Caprolactam (0, 0.023, 0.066 and 0.245 mg/l analytical conc) by whole body inhalation (aerosol), 6 hours/day, 5 days/week for		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		13 weeks plus 4 week-recovery. Post-exposure recovery period in satellite groups: An additional 10 animals/sex/group were similarly exposed and then held for a 4-week recovery period Endpoint: NOAEC = 0.066 mg/L air Critical effect: irritation (respiratory tract) **Other Tier 3:** No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of Massachusetts, New Jersey, New York and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM) and OECD HPV.		
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details	NA	**Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/07/88), no value at this time. Caprolactam has not undergone a complete evaluation and determination for evidence of human carcinogenic potential. **PPRTV:** No PPRTV record available 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)	Yes	YES-oral No-inhalation, the RfD is based on a reproductive-developmental effect. Oral Exposure Pathways- Full Term Exposure	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	Refer to RfD Details.	Refer to IRIS RfD Details. In addition, the following studies support the Serota et. al developmental effect finding: 1) Rat developmental study: oral gavage doses of 100, 500, 100 mg/kg/day on gestation days 6-20; LOAEL and NOAEL for fetal resorption is 1000 and 500		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		mg/kg/day, respectively (Gad et al., 1984). 2) Rabbit developmental study: oral gavage doses of 50, 150, 250 mg/kg/day on gestation days 6-28; LOAEL and NOAEL for reduced maternal and fetal body weight is 150 and 50 mg/kg/day, respectively (Gad et al., 1984).		
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		
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)	330	MDEQ, 2015
Target Detection Limit – Water (μg/L)	10	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