CHEMICAL UPDATE WORKSHEET

Chemical Name:	**3-Methylphenol**
CAS #:	**108-39-4**
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)	108.13	108.14	EPI	EXP
Physical State at ambient temp	Solid	Liquid	MDEQ	
Melting Point (˚C)	304	11.80	EPI	EXP
Boiling Point (˚C)	191	202.20	EPI	EXP
Solubility (ug/L)	2.80E+7	22700	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	0.3192	0.11	EPI	EXP
HLC (atm-m^3/mol at 25˚C)	1.60E-6	8.56E-007	EPI	EXP
Log Kow (log P; octanol-water)	1.99	1.96	EPI	EXP
Koc (organic carbon; L/Kg)	45.1	300.4	EPI	EXP
Ionizing Koc (L/Kg)		NA	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.074	7.08E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.3E-6	9.32E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR			

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (˚C)	178 F	86	CRC	EXP
Lower Explosivity Level (LEL; unit less)	NA	0.011	CRC	EXP
Critical Temperature (K)		705.8	CRC	EXP
Enthalpy of Vaporization (cal/mol)		11.40	CRC	EXP
Density (g/mL, g/cm^3)		1.0339	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	NA	2.23E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	NA	2.23E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	NA	2.82E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	NA	2.82E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	--	5.0E-2	IRIS, 1990	
RfD details	--	**Tier 1 Source:** **Basis:** IRIS is a Tier 1 source. **IRIS:** (09/01/1990) RfD = 5E-2 mg/kg-day. **Critical Study:** 1) U.S. EPA. 1986. o, m, p-Cresol. 90-Day oral subchronic toxicity studies in rats. Office of Solid Waste, Washington, DC. 2) U.S. EPA. 1987. o, m, p-Cresol. 90-Day oral subchronic neurotoxicity study in rats. Office of Solid Waste, Washington, DC. **Methods**: In a 90-day subchronic toxicity study (U.S. EPA, 1986), 30 Sprague-Dawley rats/sex/dose were gavaged daily with 0, 50, 150, or 450 mg/kg/day m-cresol. **Critical effect**: Decreased body weights and neurotoxicity. **Endpoint or Point of Departure (POD):** NOAEL = 50 mg/kg/day; LOAEL = 150 mg/kg/day. **Uncertainty Factors**: UF = 1,000 (10 for interspecies and 10 for intraspecies variability and 10 for uncertainty in extrapolation of subchronic data to levels of chronic effects). **Tier 1 and 2 Sources:** **EPA-OPP**: Significant toxicological residues of m-cresol and xylenol are not expected to occur in food/feed commodities from registered uses of the end-use pesticide product. Therefore, reference doses are not required. Source: USEPA-OPP Reregistration Eligibility Decision (RED) M-CRESOL AND XYLENOL. September 1994. **PPRTV:** Per PPRTV (01/31/2002), only cancer data was searched. **MRL:** No MRL record available at this time. **Tier 3 Sources:** **MDEQ:** Per DEQ-CCD/WRD RfD = 0.1 mg/kg/day based on an oral LOAEL of 30		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		mg/kg/d in Sprague-Dawley male and female rats exposed in a two-generation reproduction study (Neeper-Bradley and Tyl, 1989). UF = 300. **Critical study:** Neeper-Bradley TL, Tyl RW. 1989. Two-generation reproduction study of m-cresol (CAS No. 108-39-4) administered by gavage to Sprague-Dawley (CD®) rats. Project report 51-634. Union Carbide Corporation. Submitted to the U.S. Environmental Protection Agency under TSCA Section 4. OTS0529224. **MDEQ**: Per DEQ-CCD-RRD,02/23/1993, RfD = 0.05 based on IRIS 1990.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	
CSF details		Classification = C, possible human carcinogen based on an increased incidence of skin papilloma in mice in an initiation-promotion study. The three cresol isomers produced positive results in genetic toxicity studies both alone and in combination. Source: IRIS, 08/01/1991 **Tier 1 and 2 Sources:** **IRIS:** No value at this time. **PPRTV:** Per PPRTV (01-31-2002), A provisional oral slope factor for 3-MP cannot be derived because human and animal oral cancer data are lacking. **MRL:** NA. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD, no value at this time.		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	1.0E+2	MDEQ, 2005	
RfC/ITSL details	--	**Tier 3 Source:** **MDEQ:** **Basis:** The MDEQ (2005) value is selected as it is a newer assessment and used		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		NIOSH REL and adequate toxicity adjustments. The California and New York values are based on route extrapolated RfD value for the mixed cresols. The RIVM value is also for mixed Cresols. See details below. **Tier 1 and 2 Sources:** **IRIS:** Per IRIS (12/11/1991), insufficient data. **PPRTV:** Per PPRTV (01-31-2002), only cancer data was reviewed. **MRL:** No MRL record available at this time. **Tier 3 Sources:** **MDEQ:** Per DEQ-CCD-AQD (2/24/2005), ITSL = 100 µg/m^3 based on NIOSH REL of 10 mg/m^3 ; ITSL was calculated following Rule 232(1)(c). **California:** Inhalation chronic REL= 600 µg/m^3 of cresol mixtures (cresols, o-cresol, m-cresol, and p-cresol) . Study: USEPA. 1987. o, m, p-Cresol. 90-Day oral subchronic neurotoxicity study in rats. Office of Solid Waste. Washington, DC: U.S. EPA. Study population: Sprague-Dawley rats Exposure method: Gavage at 0, 50, 175, 450, or 600 mg/kg-day Critical effects: Decreased body weights and neurotoxicity (tremors, salivation, lacrimation, etc.) LOAEL: 175 mg/kg-day; NOAEL: 50 mg/kg-day Exposure continuity: Daily gavage Exposure duration: 90 days Uncertainty factors (UF): 300; 3 - subchronic UF, 10 - interspecies UF, 10 - Intraspecies UF USEPA Reference Dose (RfD): 0.17 mg/kg/day Route-to-route extrapolation factor: 3500 mg/m^3 per mg/kg/day Additional note: An RfD of 0.05 mg/kg/day was derived by the USEPA for both o-cresol and m-cresol (USEPA 1998a, 1998b; listed as 2-methylphenol and 3-methylphenol). In accordance with its approved methodology (OEHHA, 2000), OEHHA used a factor of 3.		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Source: OEHHA Determination of Noncancer Chronic Reference Exposure Levels Batch 2A December 2000: Chronic Toxicity Summary – Cresol Mixtures The EPA website (http://www.epa.gov/ttnatw01/hlthef/cresols.html) reported that CALEPA has established a chronic reference exposure level of 0.004 mg/m^3 for mixed cresols based on bone marrow effects in rats. **Minnesota PCA (2015):** RfC = 600 $\mu g/m^3$ is based on CALEPA (Ref.: Toxicity Values Used by MPCA for Air Toxics Comparisons). **New York DEC (2005):** RfC = 180 $\mu g/m^3$ based on route extrapolation from a reference dose for 3-methylphenol (0.05 mg/kg-day) assuming a 70 kilogram individual inhales 20 cubic meters of air per day. (Review date – 2/2005) **RIVM (2001):** TCA = 170 $\mu g/m^3$. The Tolerable Concentration in Air value is for "Cresols". Derivation details are not available. Source: RIVM Re-evaluation of human-toxicological maximum permissible risk levels. Report 71170115, 2001, p.133 **ECHA (REACH):** DNEL = 0.75 mg/m^3 (750 $\mu g/m^3$). The Derived No Effect Level value is based on a subacute inhalation study. Species: male and female Sprague-Dawley rats Target concentration: 20 ug/l of an 0.25 % solution, Exposure frequency and duration: 6 hrs./day for 14 day. Study: Aerogen Inc. (2001) Inhalation safety of phenol and m-Cresol in rodents: a fourteen day repeat dose toxicity study, study abstract as presented at ISAM Congress 2001 (unpublished). Source: ECHA REACH Dossier on m-Cresol **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 and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada and OECD HPV.		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Inhalation Unit Risk Factor (IURF) ((µg/m^3)$^{-1}$)	--	NA	MDEQ, 2015	
IURF details		Classification = C, possible human carcinogen based on an increased incidence of skin papilloma in mice in an initiation-promotion study. The three cresol isomers produced positive results in genetic toxicity studies both alone and in combination. Source: IRIS, 8/1/1991 **Tier 1 and 2 Sources:** **IRIS:** Per IRIS (8/1/1991), no value at this time. **PPRTV:** Per PPRTV (01-31-2002), no value at this time **MRL:** No MRL available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD no value available 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 or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	The MDEQ RfD is based on a reproductive study.		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/L)	--	NO	SDWA, 1976 and USEPA SMCL List	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List		
Is there an Aesthetic Value? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	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)		2.0	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)	30 (M); 25
Updated GSI value (µg/L)	30 (M); 25
Rule 57 Drinking Water Value (µg/L)	1,400

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	1,400 (2-methylphenol) 2,700 (3-methylphenol) 1,400 (4-methylphenol)	2/1998 12/1999 2/1998
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	44,000 (2-methylphenol) 89,000 (3-methylphenol) 45,000 (4-methylphenol)	2/1998 12/1999 2/1998
Wildlife Value (WV)	NA (2-methylphenol) NA (3-methylphenol) NA (4-methylphenol)	
Human Cancer Values for Drinking Water Source (HCV-drink)	NA (2-methylphenol) NA (3-methylphenol) NA (4-methylphenol)	
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA (2-methylphenol) NA (3-methylphenol) NA (4-methylphenol)	
Final Chronic Value (FCV)	76 (2-methylphenol) 71 (3-methylphenol) 25 (4-methylphenol)	9/2011 12/1999 10/2013
Aquatic maximum value (AMV)	690 (2-methylphenol) 636 (3-methylphenol) 230 (4-methylphenol)	9/2011 12/1999 10/2013
Final Acute Value (FAV)	1,400 (2-methylphenol) 1,271 (3-methylphenol) 450 (4-methylphenol)	9/2011 12/1999 10/2013

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)	1,000	MDEQ, 2015
Target Detection Limit – Water (µg/L)	30	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