CHEMICAL UPDATE WORKSHEET

Chemical Name:	**2,6-Dimethylphenol**
CAS #:	**576-26-1**
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)	122.16	122.17	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (˚C)	---	45.70	EPI	EXP
Boiling Point (˚C)	201	201.00	EPI	EXP
Solubility (ug/L)	6.14E+6	6.050E+06	EPI	EXP
Vapor Pressure (mmHg at 25˚C)	0.177	2.74E-01	HSDB	EXP
HLC (atm-m^3/mol at 25˚C)	5.02E-6	6.65E-06	EPI	EXP
Log Kow (log P; octanol-water)	2.36	2.36	EPI	EXP
Koc (organic carbon; L/Kg)	209	501.9	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm^2/s)	0.08	6.35E-02	W9	EST
Diffusivity in Water (Dw; cm^2/s)	8.0E-6	8.5445E-06	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
Flash Point (˚C)	NA	73	PC	EXP
Lower Explosivity Level (LEL; unit less)	NA	NA	NA	NA
Critical Temperature (K)		701	CRC	EXP
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm^3)		1.01	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm^2)	NA	4.57E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm^2)	NA	4.57E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm^2)	NA	5.79E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm^2)	NA	5.79E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	6.0E-4	6.0E-4	IRIS, 1988	
RfD details	Rat subchronic oral toxicity study (Veldre & Janes, 1979); NOAEL = 0.6mg/kg/day; UF = 1000; Critical effects = body weight changes and histopathological changes of internal organs (liver, spleen, & kidneys). Source: IRIS CCD/RRD date: 1/22/1986	**Tier 1 Source:** **IRIS:** **Basis:** IRIS is a Tier 1 source. IRIS (1988) RfD = 6.0E-4 mg/kg-day. **Critical Study**: Veldre, I.A. and H.J. Janes. 1979. Toxicological studies of shale oils, some of their components and commercial products. Environ. Health Perspect. 30: 141-146 **Method(s)**: White rats (unspecified number) were exposed to 0, 0.6 and 6.0 mg/kg/day isomeric 2,6-dimethylphenol orally for 8 months. **Critical effect**: body weight changes and histopathological changes of internal organs (liver, spleen and kidneys) **End point or Point of Departure (POD):** NOEL = 0.6 mg/kg/day **Uncertainty Factors**: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study) **Additional note:** Database deficiency UF was not applied even though there are no data on chronic, teratogenicity, developmental or reproductive effects. . EPA did not use database UF at that time. **Source and date:** IRIS, Last revision date - 9/7/1988. An IRIS review of toxicological studies through 2004 did not identify any significant new study. **Tier 2 Sources**: **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Source:** **MDEQ:** Per DEQ-CCD (1/22/1986), RRD adopted IRIS value. See Part 201 Value RfD details.		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day)$^{-1}$)	--	NA	MDEQ, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
CSF details	NA	**Carcinogen Weight-of-Evidence (WOE) Class**: 2,6-Dimethylphenol has not been evaluated under EPA's IRIS program for evidence of human carcinogenic potential **Source and Date**: IRIS, 9/7/1988. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/7/1988), no value at this time. **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
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	2.0E+0	2.0E+0	MDEQ, 2002	
RfC/ITSL details	ITSL based on EPA's RfD as calculated under R232(1)(b). The RfD is based on Velder and Janes (1979). See IRIS for additional details on how the RfD was obtained. CCD/AQD date: 1/10/2002.	**Tier 3 Source:** **MDEQ:** **Basis:** MDEQ value based on extrapolated IRIS oral RfD from an 8-month oral study in rats. ECHA (REACH) value is based on an inhalation subacute (14 day) study. See details below. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/7/1988), no RfC value at this time. **PPRTV:** No PPRTV record available at this time. **MRL:** No MRL record available at this time. **Tier 3 Sources:** **MDEQ:** AQD (2002) ITSL = 2.0E+0 µg/m³ with 24 hour averaging time. **Basis:** based on IRIS (9/7/1988) RfD = 6.0E-4 mg/kg-day modified to an inhalation value using 70 kg body weight and 20 m^3/day inhalation rate. **IRIS RfD derivation:**		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Critical Study: Veldre, I.A. and H.J. Janes. 1979. Toxicological studies of shale oils, some of their components and commercial products. Environ. Health Perspect. 30: 141-146 **Method(s)**: White rats (unspecified number) were exposed to 0, 0.6 and 6.0 mg/kg/day isomeric 2,6-dimethylphenol orally for 8 months. **Critical effect**: body weight changes and histopathological changes of internal organs (liver, spleen and kidneys) **End point or Point of Departure (POD):** NOEL = 0.6 mg/kg/day **Uncertainty Factors**: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study) **Additional note:** Database deficiency UF was not applied even though there are no data on chronic, teratogenicity, developmental or reproductive effects. EPA did not use database UF at that time. **Source and date:** MDEQ-CCD/AQD, 1/10/2002 **ECHA:** Derived No Effect Level (DNEL)= 1.7E+3 µg/m^3. This value is for a Worker scenario; no DNEL for general population is available. Key study: Study report, 1991 Method: Subacute study; Male and female rats were treated with 2,6-xylenol (67, 200, 670 mg/m3) by whole body inhalation for 6 hours/day, 5 days/week, for a total of ten exposure, conducted within 14 days. Critical effect: reduced body weight and red nasal discharge upon exposure which was deemed indicative of upper respiratory tract irritation and ulceration. This was supported by histopathology. Dose descriptor starting point: NOAEC – 200 mg/m3 Overall assessment factor (AF): 300 (details not specified). Source: ECHA REACH Dossier on 2,6-Xylenol **Other Tier 3 Sources:** 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, New York, and Texas, WHO		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		(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	**Carcinogen Weight-of-Evidence (WOE) Class**: 2,6-Dimethylphenol has not been evaluated under EPA's IRIS program for evidence of human carcinogenic potential **Source and Date**: IRIS, 9/7/1988. **Tier 1 and 2 Sources**: **IRIS:** Per IRIS (9/7/1988), no value at this time. **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)	No	No. The RfD or RfC/ITSL is 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 (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)	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)	4	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