



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Xylenes
CAS #:	1330-20-7
Revised By:	RRD Toxicology Unit
Revision Date:	August 19, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	106.17	106.17	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	---	13.25	EPI	EXP
Boiling Point (°C)	137	138.23	EPI	EXP
Solubility (ug/L)	1.86E+5	106000	PP	EXP
Vapor Pressure (mmHg at 25°C)	8.36	7.99E+00	PP	EXP
HLC (atm-m³/mol at 25°C)	6.04E-3	6.63E-03	PP	EXP
Log Kow (log P; octanol-water)	3.11	3.16	PP	EXP
Koc (organic carbon; L/Kg)	348	382.9	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.078	6.91E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	3.21E-5	8.56E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	NA	27	CRC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.009	CRC	EXP
Critical Temperature (K)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm ³)		0.8801	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	2.49E-05	2.69E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	5.31E-05	6.16E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	3.49E-05	4.24E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	7.19E-05	9.47E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.8E+0	2.0E-1	ATSDR, 2014	
RfD details	<p>Chronic rat gavage study; NOAEL = 250 mg/kg --->179 mg/kg*; LOAEL = 500 mg.kg ----> 357 mg/kg*; Critical effects = hyperactivity, decreased body weight and increased mortality. UF = 100 (NTP, 1986); *Adjusted for gavage schedule (5/7). CCD/RRD date: 3/19/1987</p>	<p>Tier 2 Source: ATSDR: Basis: The ATSDR RfD is selected as the best available value because the assessment was more recent than the IRIS review. However, the RfD value and methodology is exactly the same for both the ATSDR MRL and the IRIS RfD. MRL: Per ATSDR (12/2014), chronic oral MRL = 2.0E-1 mg/kg-day derived as follows: Critical Study: NTP. 1986. National Toxicology Program technical report on the toxicology and carcinogenesis studies of xylenes (mixed) (60% m-xylene, 14% p-xylene, 9% o-xylene, and 17% ethylbenzene) (CAS No. 1330-20-7) in F344/N rats and B6C3F1 mice (gavage studies). Research Triangle Park, NC: U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program. NTP TR 327. NIH Publication No. 87-2583. Method(s): Fischer 344 rats (50/sex/group) were exposed to mixed xylenes (60% m-xylene, 13.6% p-xylene, 9.1% o-xylene, 17.0% ethylbenzene) in corn oil by gavage at doses of 0, 250, or 500 mg/kg-day, 5 days/week for 103 weeks. Critical effect: decreased survival in male rats End point or Point of Departure (POD): NOAEL = 250 mg/kg; duration adjusted NOAEL = 179 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation, and database deficiencies) Additional Note: A single chronic-duration oral MRL has been derived based on data for mixed xylenes that applies to mixed xylenes and all of the individual isomers. The justification for deriving a common value is that the isomers have similar toxicokinetic properties and elicit similar toxicological effects, with no isomer consistently exhibiting the greatest potency, depending on the end point. Source and date: ATSDR, 8/2007 (from ATSDR 12/2014 list)</p> <p>Tier 1 and 2 Sources:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>IRIS:</p> <p>Critical Study: NTP (National Toxicology Program). (1986) NTP technical report on the toxicology and carcinogenesis of xylenes (mixed) (60% m-xylene, 13.6% p-xylene, 17.0% ethylbenzene, and 9.1% o-xylene) in F344/N rats and B6C3F1 mice (gavage studies). Research Triangle Park, NC. NTP TR 327, NIH Publ. No. 86-2583.</p> <p>Methods: Fischer 344 rats (50/sex/group) and B6C3F1 mice (50/sex/group) were exposed to mixed xylenes (60% m-xylene, 13.6% p-xylene, 9.1% o-xylene, 17.0% ethylbenzene) in corn oil by gavage at doses of 0, 250, or 500 mg/kg-day (rats) and 0, 500, or 1000 mg/kg-day (mice) for 5 days per week for 103 weeks.</p> <p>Critical effect: decreased body weight and increased mortality in the high-dose male rats</p> <p>End point or Point of Departure (POD): NOAEL = 179 mg/kg-day NOAEL_{ADJ} = 250 mg/kg-day (corrected for 5/7 days dosing schedule)</p> <p>Uncertainty Factors: UF = 1000 (10 each for intraspecies variability, interspecies extrapolation, and database uncertainty)</p> <p>Source and date: IRIS, Last revision date - 2/21/2003. An IRIS Toxicological Review is available.</p> <p>PPRTV: PPRTV (9/30/2009) refers to the IRIS RfD value. A subchronic p-RfD of 0.4 mg/kg-day is available.</p> <p>Tier 3 Source:</p> <p>MDEQ: Per DEQ-CCD/WRD (9/15/2010), RfD = 1.8E+0 mg/kg-day.</p> <p>Critical Study: NTP. 1986. National Toxicology Program technical report on the toxicology and carcinogenesis studies of xylenes (mixed) (60% m-xylene, 14% p-xylene, 9% o-xylene, and 17% ethylbenzene) (CAS No. 1330-20-7) in F344/N rats and B6C3F1 mice (gavage studies). Research Triangle Park, NC: U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program. NTP TR 327. NIH Publication No. 87-2583.</p> <p>Methods: Fischer 344 rats (50/sex/group) were exposed to mixed xylenes (60%</p>		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		m-xylene, 13.6% p-xylene, 9.1% o-xylene, 17.0% ethylbenzene) in corn oil by gavage at doses of 0, 250, or 500 mg/kg-day, 5 days/week for 103 weeks. Critical effect: decreased survival in male rats End point or Point of Departure (POD): NOAEL = 250 mg/kg; duration adjusted NOAEL = 179 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation, and database deficiencies) Source and date: MDEQ-CCD/WRD, 9/15/2010		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	Carcinogen Weight-of-Evidence (WOE) Class: inadequate for an assessment of the carcinogenic potential of xylenes. IRIS WOE Basis: Adequate human data on the carcinogenicity of xylenes are not available, and the available animal data are inconclusive as to the ability of xylenes to cause a carcinogenic response. Evaluations of the genotoxic effects of xylenes have consistently given negative results. Source and Date: IRIS, Last revision date - 2/21/2003. An IRIS Toxicological Review is available. Tier 1 and 2 Sources: IRIS: No value available. PPRTV: Per PPRTV (9/30/2009), no value at this time. MRL: NA; MRLs are for non-cancer effects only.		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	4.4E+3	2.2E+2	ATSDR, 2007	
RfC/ITSL details	Based on EPA's 2/21/03 RfC. Rat behavioral	Tier 2 Source: ATSDR: Basis: ATSDR, is a Tier 1 source. The MRL RfC was selected because it is based on		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	<p>changes in a sub-chronic inhalation study reported by Korsak et al (1994). NOAEL of 50 ppm, LOAEL 100 ppm, exposure to m-xylene caused rotarod performance changes.</p> <p>NOAEL_(adj) = NOAEL_(hec) = 39 mg/m³. An uncertainty factor of 300 was applied to NOAEL_(hec) to obtain the RfC. See IRIS 2003 printout for additional details. CCD/AQD date: 3/31/2003</p>	<p>human data.</p> <p>Chronic inhalation MRL = 0.05 ppm (2.2E+2 µg/m³, where 1 ppm = 4.34 mg/m³) is derived as follows:</p> <p>Critical Study(ies): Uchida Y, Nakatsuka H, Ukai H, et al. 1993. Symptoms and signs in workers exposed predominantly to xylenes. Int Arch Occup Environ Health 64:597-605.</p> <p>Method(s): 175 workers (107 men, 68 women) were exposed to mixed xylenes in Chinese factories during the production of rubber boots or plastic coated wire, or in printing work. Nonexposed workers (116 men, 125 women) were recruited from the same or other factories as a comparison population. Exposures, measured with a diffusive sampler, indicated that xylenes accounted for >70% total exposure, with m-xylene accounting for 50% of the xylene exposure, followed by p- and o-xylenes. Toluene exposure and ethylbenzene exposure were about 1 and 3 ppm, respectively, with no benzene exposure.</p> <p>Critical effect: subjective symptoms of neurotoxicity (anxiety, forgetfulness, floating sensation) and respiratory toxicity (nasal irritation and sore throat) and eye irritation. These symptoms were observed in Ernstgard et al (2002), the principal study used for deriving the acute-duration inhalation exposure MRL</p> <p>End point or Point of Departure (POD): LOAEL = 14 ppm</p> <p>Uncertainty Factors: UF = 300 (10 each for intraspecies variability and use of a LOAEL and 3 for database deficiencies)</p> <p>Additional note: Note: A single chronic-duration inhalation MRL has been derived based on data for mixed xylene that applies to mixed xylenes and all of the individual isomers. The justification for deriving a common value is that the isomers have similar toxicokinetic properties and elicit similar toxicological effects, with no isomer consistently exhibiting the greatest potency, depending on the end point.</p> <p>Source and date: ATSDR, 8/2007</p> <p>Tier 1 and 2 Sources:</p> <p>IRIS: RfC = 0.1 mg/m³ = 1.0E+2 µg/m³</p> <p>Critical Study(ies): Korsak, Z., J.A. Sokal and R. Gómy. 1992. Toxic effects of</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>combined exposure to toluene and m-xylene in animals. III. Subchronic inhalation study. Pol. J. Occup. Med. Environ. Health. 5(1):27–33.</p> <p>Method(s): Male Wistar rats (12/dose) were exposed to toluene, m-xylene, or a 1:1 mixture for 6 hours per day, 5 days per week at a concentration of 0 or 100 ppm for 6 months or 1000 ppm for 3 months.</p> <p>Critical effect: Impaired motor coordination (decreased rotarod performance)</p> <p>End point or Point of Departure (POD): NOAEL = 50 ppm; NOAEL_(HEC) = 39 mg/m³ ; LOAEL = 100 ppm (LOAEL_(HEC) = 78 mg/m³)</p> <p>Uncertainty Factors: UF = 300 (10 for intraspecies variability and 3 each for interspecies extrapolation, use of a subchronic study, and database deficiencies)</p> <p>Source and date: IRIS, Last revision date - 2/21/2003. An IRIS Toxicological Review is available.</p> <p>PPRTV: PPRTV (9/30/2009) refers to the IRIS RfC. A subchronic p-RfC of 0.4 mg/m³ is available.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD (3/31/2003), AQD adopted the IRIS RfC.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: inadequate for an assessment of the carcinogenic potential of xylenes.</p> <p>IRIS WOE Basis: Adequate human data on the carcinogenicity of xylenes are not available, and the available animal data are inconclusive as to the ability of xylenes to cause a carcinogenic response. Evaluations of the genotoxic effects of xylenes have consistently given negative results.</p> <p>Source and Date: IRIS, Last revision date - 2/21/2003. An IRIS Toxicological Review is available.</p> <p>Tier 1 and 2 Sources: IRIS: No value available. PPRTV: Per PPRTV (9/30/2009), no value at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		MRL: NA; MRLs are for non-cancer effects only.		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2014	
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, 2014	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (ug/L)	10,000	10,000	SDWA, 1976	
SDWS details	SDWA, 1976	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)	YES	YES	MDEQ, 1991	
Aesthetic value (ug/L)	280	280	MDEQ, 1991	
Aesthetic Value details	Same as →	Aesthetic criteria via odor testing derived for Michigan DNR by ABB Environmental Services, 1991. See electronic and hard file for a copy of the 1991 document titled, "Determination of Threshold Odor Numbers for Six Substances prepared for the MDNR", December 1991.		
Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Phytotoxicity details	NA	NA	NA	
Others	--	--		

(C) Chemical-specific Exposure Factors

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS _{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS _{gi} details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (A _{Ed})	---	0.1	MDEQ, 2015	
A _{Ed} details				
Ingestion Absorption Efficiency (A _{Ei})		1.0	MDEQ, 2015	
A _{Ei} 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)	41
Updated GSI value (µg/L)	41
Rule 57 Drinking Water Value (µg/L)	3,800

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	3,800	9/2010
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	16,000	9/2010
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	NA
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	NA
Final Chronic Value (FCV)	41	9/2005
Aquatic maximum value (AMV)	370	9/2005
Final Acute Value (FAV)	730	9/2005

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)

(E) Analytical Information

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	150	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	3	MDEQ, 2015
Target Detection Limit – Air (ppbv)	2.30E+01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	7.60E+02	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