



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Toluene</b>
<b>CAS #:</b>	<b>108-88-3</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	August 19, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	92.14	92.14	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	---	-94.90	EPI	EXP
Boiling Point (°C)	110.6	110.60	EPI	EXP
Solubility (ug/L)	5.26E+5	526000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	28.12	2.84E+01	EPI	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	6.64E-3	6.64E-03	EPI	EXP
Log Kow (log P; octanol-water)	2.75	2.73	EPI	EXP
Koc (organic carbon; L/Kg)	180	233.9	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.087	7.78E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	8.6E-6	9.20E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	40 F	4	CRC	EXP
Lower Explosivity Level (LEL; unitless)	0.011	0.011	CRC	EXP
Critical Temperature (K)		5.92E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		7.93E+03	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.8623	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.57E-05	2.73E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	5.81E-05	6.39E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	3.62E-05	4.32E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	8.02E-05	9.93E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
<b>Reference Dose (RfD) (mg/kg/day)</b>	2.2E-1	7.9E-2	IRIS, 2005	
<b>RfD details</b>	<p>NOAEL = 312 mg/kg; LOAEL = 625 mg/kg; Critical effect = changes in liver and kidney weights. 13-week gavage study (5/7d). (NTP, 1989); UF = 1000</p> <p>CCD/RRD date: 6/20/1990</p>	<p><b>Tier 1 Source:</b>  <b>IRIS:</b>  <b>Basis:</b> IRIS is a Tier 1 source.  <b>IRIS RfD=</b> 7.9E-2 mg/kg/day  <b>Critical Study:</b> NTP (National Toxicology Program). (1990) Toxicology and carcinogenesis studies of toluene (CAS No. 108-88-3) in F344/N rats and B5C3F1 mice (inhalation studies). Public Health Service, U.S. Department of Health and Human Services; NTP TR 371. Available from: National Institute of Environmental Health Sciences, Research Triangle Park, NC.  <b>Method(s):</b> Male and female F-344 rats and B6C3F1 mice were exposed to toluene by gavage (in corn oil) for 13 weeks. Groups of 10 rats/sex/group were exposed to 0, 312, 625, 1250, 2500 or 5000 mg/kg toluene, 5 days/week for 13 weeks. The exposure, adjusted to a 7-day week resulted in dose estimates of 0, 223, 446, 893, 1786 or 3571 mg/kg-day, respectively.  <b>Critical effect(s):</b> increased kidney weight  <b>End point or Point of Departure (POD):</b> BMDL = 238 mg/kg-day  <b>Uncertainty Factors:</b> UF = 3,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study, and 3 for database insufficiencies).  <b>Source and date:</b> IRIS, Last revision date - 9/23/2005</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV:</b> PPRTV (9/29/2009) refers to IRIS RfD. A <u>subchronic</u> p-RfD = 8.0E-1 was derived based on the NTP (1990) study used for deriving the IRIS value.  <b>MRL:</b> Per ATSDR List (4/2015), no oral chronic MRL value at this time. Oral intermediate MRL = 2.0E-2 mg/kg-day was derived as follows:  <b>Critical Study:</b> Hsieh GC, Sharma RP, Parker RDR et al. 1990b. Evaluation of toluene exposure via drinking water on levels of regional brain biogenic monoamines and their metabolites in CD-1 mice. Ecotox Environ Safety 20: 175–184.</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Method(s):</b> Male CD-1 mice (5/group) were exposed to toluene in drinking water for 28 days. The estimated toluene treatment doses are 0, 5, 22, and 105 mg/kg/day based on water consumption and average toluene concentrations.</p> <p><b>Critical effect:</b> neurological effects</p> <p><b>End point or Point of Departure (POD):</b> LOAEL = 5 mg/kg-day</p> <p><b>Uncertainty Factors:</b> UF = 300 (10 each for intraspecies variability and interspecies extrapolation, and 3 for use of a LOAEL).</p> <p><b>Source and date:</b> ATSDR, final 9/2000</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/RRD (6/20/1990), RfD = 2.2E-1 mg/kg-day. See Part 201 Value RfD details.</p>		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	--	NA	MDEQ, 2015	
<b>CSF details</b>	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "inadequate information to assess the carcinogenic potential"</p> <p><b>IRIS WOE Basis:</b> studies of humans chronically exposed to toluene are inconclusive, toluene was not carcinogenic in adequate inhalation cancer bioassays of rats and mice exposed for life (CIIT, 1980; NTP, 1990; Huff, 2003), and increased incidences of mammary cancer and leukemia were reported in a lifetime rat oral bioassay at a dose level of 500 mg/kg-day but not at 800 mg/kg-day (Maltoni et al., 1997).</p> <p><b>Source and Date:</b> IRIS, 9/23/2005</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (9/23/2005), no value at this time.  <b>PPRTV:</b> Per PPRTV (9/29/2009), no value at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD, no value at this time</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>	4.0E+2	5.0E+3	IRIS, 2005	
<b>RfC/ITSL details</b>	<p>Per AQD: ITSL based on EPA's RfC of 0.1 <math>\mu\text{g}/\text{m}^3</math>. The RfC based on human occupational data effects were neurological and changes in nasal epithelium, Foo et al 1990. CCD/AQD date: 8/4/1992.</p>	<p><b>Tier 1 Source:</b> <b>IRIS:</b> <b>Basis:</b> IRIS is a Tier 1 source. <b>IRIS RfC=</b> 5.0E+3 <math>\mu\text{g}/\text{m}^3</math> <b>Critical Study:</b> Multiple occupational human studies: Abbate et al. (1993); Boey et al. (1997); Cavalleri et al. (2000); Eller et al. (1999); Foo et al. (1990); Murata et al. (1993); Nakatsuka et al. (1992); Neubert et al. (2001); Vrca et al. (1995) and; Zavalic et al. (1998). <b>Methods:</b> An arithmetic mean of the NOAEL values derived from the principal studies (refer to Table 1 of IRIS Toxicological Review) was chosen to represent an average point of departure. The highest NOAEL was identified as 44 ppm (Nakatsuka et al., 1992). The lowest LOAELs were identified as 40-42 ppm (Vrca et al., 1995, 1997; Cavalleri et al., 2000). The average exposure level of 34 ppm is used as the point of departure for the RfC. <b>Critical effect:</b> neurological effects in occupationally-exposed workers <b>End point or Point of Departure (POD):</b> NOAEL (average) = 34 ppm (128 <math>\text{mg}/\text{m}^3</math>); NOAEL<sub>ADJ</sub> = 46 <math>\text{mg}/\text{m}^3</math> <b>Uncertainty Factors:</b> UF = 10 for intraspecies variability <b>Source and date:</b> IRIS, Last revision date - 9/23/2005</p> <p><b>Tier 2 Sources:</b> <b>PPRTV:</b> PPRTV (9/29/2009) refers to IRIS RfC. <b>MRL:</b> Per ATSDR List (4/2015), inhalation chronic MRL = 0.08 ppm (0.3 <math>\text{mg}/\text{m}^3</math>) derived as follows: <b>Critical Study:</b> 1) Zavalic, M, Mandic, Z, Turk, R et al. 1998a. Quantitative assessment of color vision impairment in workers exposed to toluene. Am J Ind Med 32: 297-304.; and 2) Zavalic, M, Mandic, Z, Turk, R et al. 1988c. Assessment</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>of color vision impairment in male workers exposed to toluene generally above occupational exposure limits. Occup Med 48(3):175-180</p> <p><b>Method(s):</b> Three groups of Croatian workers were examined by means of interviews, medical examination, and color vision testing using the Lanthony 15 Hue desaturated panel in standard conditions. The first group consisted of 46 workers (43 women and 3 men) employed in manually gluing shoe soles and exposed to median of 32 ppm and geometric mean levels of 35 ppm toluene. The second group consisted of 37 workers (34 men and 3 women) employed in a rotogravure printing press and exposed to median levels of 132 ppm and geometric mean levels of 156 ppm toluene. The third group consisted of 90 workers (61 men and 29 women) not occupationally exposed to any solvents or known neurotoxic agents. The average age of the workers was 41 years.</p> <p><b>Critical effect:</b> color vision impairment</p> <p><b>End point or Point of Departure (POD):</b> LOAEL = 35 ppm; LOAEL<sub>ADJ</sub> = 35 ppm x 5 days/7 days x 8 hours/24 hours</p> <p><b>Uncertainty Factors:</b> UF = 100 (10 each for intraspecies variability and use of a LOAEL).</p> <p><b>Source and date:</b> ATSDR, 9/2000</p> <p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b> Per DEQ-CCD (9/27/2005), AQD adopted the IRIS RfC value.</p>		
<b>Inhalation Unit Risk Factor (IURF) ((<math>\mu\text{g}/\text{m}^3</math>)<sup>-1</sup>)</b>	--	NA	MDEQ, 2015	
<b>IURF details</b>	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "inadequate information to assess the carcinogenic potential"</p> <p><b>IRIS WOE Basis:</b> studies of humans chronically exposed to toluene are inconclusive, toluene was not carcinogenic in adequate inhalation cancer bioassays of rats and mice exposed for life (CIIT, 1980; NTP, 1990; Huff, 2003), and increased incidences of mammary cancer and leukemia were reported in a lifetime rat oral bioassay at a dose level of 500 mg/kg-day but not at 800 mg/kg-day (Maltoni et al., 1997).</p> <p><b>Source and Date:</b> IRIS, 9/23/2005</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (9/23/2005), no value at this time. <b>PPRTV:</b> Per PPRTV (9/29/2009), no value at this time. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time.		
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	NO	USEPA, 2015	
<b>MMOA Details</b>	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	No. The RfD nor ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<b>State Drinking Water Standard (SDWS) (ug/L)</b>	1.0E+3	1.0E+3	SDWA, 1976	
<b>SDWS details</b>	SDWA, 1976	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (ug/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
<b>Is there an aesthetic value for drinking water? (Y/N)</b>	YES	YES		
<b>Aesthetic value</b>	7.9E+2	7.9E+2	MDNR/ABB, 1991	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(ug/L)				
<b>Aesthetic Value details</b>		Determination of Threshold Odor Numbers for Six Substances. Prepared for MDNR. December 1991. ABB Environmental Services, Inc.		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA	NA	
<b>Others</b>	--	--		

**(C) Chemical-specific Exposure Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS <sub>gi</sub> details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (A <sub>Ed</sub> )	---	0.1	MDEQ, 2015	
A <sub>Ed</sub> details				
Ingestion Absorption Efficiency (A <sub>Ei</sub> )		1.0	MDEQ, 2015	
A <sub>Ei</sub> Details				
Relative Source Contribution for Water (RSC <sub>w</sub> )		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC <sub>s</sub> )		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC <sub>A</sub> )		1.0	MDEQ, 2015	
Others				

**(D) Rule 57 Water Quality Values and GSI Criteria**

<b>Current GSI value (µg/L)</b>	270
<b>Updated GSI value (µg/L)</b>	270
<b>Rule 57 Drinking Water Value (µg/L)</b>	5,600

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	5,600	7/1997
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	51,000	7/1997
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	NA	NA
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	NA	NA
<b>Final Chronic Value (FCV)</b>	270	7/2013
<b>Aquatic maximum value (AMV)</b>	1,300	7/2013
<b>Final Acute Value (FAV)</b>	2,600	7/2013

Sources:

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

**(E) Analytical Information**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	100	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	1	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	1.30E+03	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	4.40E+04	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