



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>o-Chlorotoluene</b>
<b>CAS #:</b>	<b>95-49-8</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	January 5, 2016

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	126.58	126.59	EPI	EXP
Physical State at ambient temp	Liquid	Liquid		
Melting Point (°C)	---	-35.60	EPI	EXP
Boiling Point (°C)	158.97	159.00	EPI	EXP
Solubility (ug/L)	3.73E+5	3.74E+05	EPI	EXP
Vapor Pressure (mmHg at 25°C)	3.43	3.43E+00	EPI	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	3.57E-3	3.57E-03	EPI	EXP
Log Kow (log P; octanol-water)	3.42	3.42	EPI	EXP
Koc (organic carbon; L/Kg)	612	382.9	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.08	6.29E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	8.0E-6	8.7194E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	96 F	35.6	NPG	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.01	PC	EXP
Critical Temperature (K)		654.25	HSDB	EXP
Enthalpy of Vaporization (cal/mol)		8.96E+03	CRC	EXP
Density (g/mL, g/cm <sup>3</sup> )		1.0825	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	8.30E-06	2.63E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	1.77E-05	5.78E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	1.16E-05	4.11E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	2.40E-05	8.72E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	2.0E-2	6.7E-3	PPRTV, 2010/MDEQ, 2015	
RfD details	NOAEL=20 mg/kg/d, 15-week rat oral exposure study (gavage), UF=1000. Critical effect = decrease in body weight (Gibson et al., 1974). Entry date: 09/21/1989	<p><b>Tier 2 Source:</b>  <b>PPRTV:</b>  <b>Basis:</b> PPRTV (9/30/2010) subchronic p-RfD = 0.02 mg/kg-day. MDEQ applied an additional UF of 3 to account for subchronic to chronic extrapolation and to cap the UF to 3,000 per EPA guidance. The final chronic RfD = 0.002 mg/kg-day. The PPRTV subchronic p-RfD is the same as the IRIS chronic RfD of 2.0E-2. Both use the same study and POD; however IRIS did not apply a database UF even though the database was rated low due to lack of chronic, reproductive and developmental toxicity studies. IRIS, at that time, did not consider UF for database.  <b>Critical Study:</b> Gibson, W.R., F.O. Gossett, G.R. Koenig and F. Marroquin. 1974a. The toxicity of daily oral doses of o-chlorotoluene in the rat. Toxicology Division, Lilly Research Laboratories. Submitted to Test Rules Development Branch, Office of Toxic Substances, U.S. EPA, Washington D.C. (unpublished)  <b>Method(s):</b> Weanling Harlan rats (20 sex/dose) were exposed to 0, 20, 80, or 320 mg/kg/day o-chlorotoluene in an aqueous solution containing 5% acacia by gavage for 103 or 104 days.  <b>Critical effect:</b> decreased body weight gain and absolute body weight in male rats  <b>End point or Point of Departure (POD):</b> NOAEL = 20 mg/kg-day  <b>Uncertainty Factors:</b> PPRTV UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and database deficiencies).</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (2/1/1990), RfD = 2.0E-2 mg/kg-day:  <b>Critical Study:</b> Gibson, W.R., F.O. Gossett, G.R. Koenig and F. Marroquin. 1974a. The toxicity of daily oral doses of o-chlorotoluene in the rat. Toxicology Division, Lilly Research Laboratories. Submitted to Test Rules Development Branch, Office of Toxic Substances, U.S. EPA, Washington, D.C. (unpublished)</p>		COMPLETE



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Method(s):</b> Weanling Harlan rats (20 sex/dose) were exposed to 0, 20, 80, or 320 mg/kg/day o-chlorotoluene in an aqueous solution containing 5% acacia by gavage for 103 or 104 days.</p> <p><b>Critical effect:</b> decreased body weight gain and absolute body weight in male rats</p> <p><b>End point or Point of Departure (POD):</b> NOAEL = 20 mg/kg-day</p> <p><b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and database deficiencies)</p> <p><b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/RRD; RfD is the same as the IRIS RfD. 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 Carcinogenic Potential"</p> <p><b>IRIS WOE Basis:</b> There is not adequate information available to assess carcinogenic potential.</p> <p><b>Source and Date:</b> PPRTV, 9/30/2010</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (2/1/1990), no value at this time.  <b>PPRTV:</b> Per PPRTV (9/30/2010), 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
<b>Reference Concentration (RfC) or Initial</b>	7.0E+1	8.0E+1	CALEPA, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
<b>Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>				
<b>RfC/ITSL details</b>	<p>AQD staff initially evaluated this compound in 1994 using interim ITSL procedures to derive a permissible impact of 2590 <math>\mu\text{g}/\text{m}^3</math> and 70 <math>\mu\text{g}/\text{m}^3</math> for an 8 hr. and 24 hr. averaging time, respectively. The RIS oral reference dose (RfD) of 0.02 mg/kg/day for OCT was based on a 15-week oral gavage study in rats. A total of 20 Harlan rats/sex/group were dosed at 0, 20, 80, or 320 mg/kg/day for 104 days. At doses of 80 and 320 mg/kg/day,</p>	<p><b>Tier 3 Source:</b>  <b>CALEPA:</b>  <b>Basis:</b> CALEPA-DTSC uses the more current OSWER 80 kg body weight and is not a screening value. CAL chronic RfC is preferred over PPRTV's subchronic screening value. See details below.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (2/1/1990), no value at this time.</p> <p><b>PPRTV:</b> Subchronic screening RfC = <math>8.0\text{E-}1 \text{ mg}/\text{m}^3</math>  <b>Critical Studies:</b> Edwards, J.A. et al. (1982) Effect of 2-chlorotoluene vapor on pregnancy of the rat. Department of Inhalation Toxicology, Huntingdon Research Center, December 31, 1982. OTS0507455 Unpublished (Occidental, 1983, 594423) (unpublished)  <b>Method(s):</b> groups of 25 time-mated Sprague-Dawley female rats were exposed via whole-body inhalation to 0, 1, 3, or 9 mg/L o-chlorotoluene for 6 hours per day during gestation days (GD) 6–19. Concentration equivalents are 0, 250, 750, or 2250 <math>\text{mg}/\text{m}^3</math> after duration and concentration adjustments.  <b>Critical effect:</b> Maternal toxicity (slight ataxia, decreased body-weight gains and food consumption, and increased water consumption) LOAEL at 3 mg/l (250 <math>\text{mg}/\text{m}^3</math>). At 9 mg/L (750 <math>\text{mg}/\text{m}^3</math>), decreased fetal mean litter weight and mean fetal weight and increased incidence (6 fetuses; 4 litters) of brachydactyly were observed.  <b>End point or Point of Departure (POD):</b> <math>\text{NOAEL}_{\text{HEC}} = 250 \text{ mg}/\text{m}^3</math>  <b>Uncertainty Factors:</b> PPRTV UF = 300 (10 each for intraspecies variability and database deficiencies; and 3 for interspecies extrapolation to account for the toxicodynamic portion). MDEQ used an additional UF of 10 to account for the use of a subchronic study; total UF = 3,000.  <b>Source and date:</b> PPRTV (Appendix A), 9/30/2010</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	<p>male rats developed a statistically significant decrease in mean body weight gain and an increase in adrenal weight. Additionally at the 80 mg/kg/day dose, blood urea nitrogen was increased in males. No histological changes related to intake of OCT were seen in this investigation. A NOAEL (no-observable-adverse-effect-level) of 20 mg/kg/day was indicated for this study which resulted in a RfD of 0.2 mg/kg/day. This RfD resulted in an ITSL of 70 ug/m<sup>3</sup> 24 hr.</p>	<p><b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ:</b> Per DEQ-CCD/AQD (4/17/2001), ITSL = 7.0E+1 µg/m<sup>3</sup>. This value is based on the IRIS RfD and 70 ug/m<sup>3</sup> body weight for an 8-hour and 24-hour averaging time.  <b>Critical Study:</b> Gibson, W.R., F.O. Gossett, G.R. Koenig and F. Marroquin. 1974a. The toxicity of daily oral doses of o-chlorotoluene in the rat. Toxicology Division, Lilly Research Laboratories. Submitted to Test Rules Development Branch, Office of Toxic Substances, U.S. EPA, Washington, D.C. (unpublished)  <b>Method(s):</b> Weanling Harlan rats (20 sex/dose) were exposed to 0, 20, 80, or 320 mg/kg/day o-chlorotoluene in an aqueous solution containing 5% acacia by gavage for 103 or 104 days.  <b>Critical effect:</b> decreased body weight gain and absolute body weight in male rats  <b>End point or Point of Departure (POD):</b> NOAEL = 20 mg/kg-day  <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and database deficiencies)</p> <p><b>California DTSC 2015 (CALEPA):</b> RfC = 8.0E+1 µg/m<sup>3</sup>. Oral route extrapolation from IRIS (1990) RfD 2.0E-2 mg/kg/day. Uses 80 kg body weight. See IRIS RfD details.</p> <p><b>Texas CEQ 2015:</b> RfC = 8.0E-1 mg/m<sup>3</sup> = 800 µg/m<sup>3</sup>. Based on PPRTV 2010 screening value.</p> <p><b>ECHA (REACH):</b> DNEL (Derived No Effect Level) = 0.86 mg/m<sup>3</sup>. No critical study reference available. Methods: Rabbits were exposed to 2 -chlorotoluene vapor (4.0, 7.8, 11.5 or 15.6 mg/l analytic concentration) over a period of 23 consecutive days for daily 6 hours. LOAEL = ca. 8 mg/l/d (6 hours/day). No further information available.</p>		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	averaging time. CCD/AQD date: 4/17/2001	<b>Other Tier 3:</b> No value is available from these sources: HEAST 1997, NTP ROC, Massachusetts DEP 2015, Minnesota 2015, New Jersey DEP 2011, New York DEP 2006, WHO (IARC and IPCS/INCHEM), Canada, RIVM, OECD HPV		
<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 Carcinogenic Potential"</p> <p><b>IRIS WOE Basis:</b> There is not adequate information available to assess carcinogenic potential.</p> <p><b>Source and Date:</b> PPRTV, 9/30/2010</p> <p><b>Tier 1 and 2 Sources:</b></p> <p><b>IRIS:</b> Per IRIS (2/1/1990), no value at this time.</p> <p><b>PPRTV:</b> Per PPRTV (9/30/2010), no value at this time.</p> <p><b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b></p> <p><b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		Complete
<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 RfC or RfD is not based on a reproductive-developmental effect.		MDEQ, 2015
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<b>State Drinking Water Standard</b>	--	NO	SDWA, 1976	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(SDWS) (ug/L)				
<b>SDWS details</b>	NA	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>	NO	NO	NA	
<b>Aesthetic value (ug/L)</b>	NO	Not evaluated.	NA	
<b>Aesthetic Value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA	NA	
<b>Others</b>				

**(C) Chemical-specific Absorption 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 (AE <sub>d</sub> )	---	0.1	MDEQ, 2015	
AE <sub>d</sub> details				
Ingestion Absorption Efficiency (AE <sub>i</sub> )		1.0	MDEQ, 2015	
AE <sub>i</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>	ID
<b>Updated GSI value (µg/L)</b>	ID
<b>Rule 57 Drinking Water Value (µg/L)</b>	360

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	360	10/2000
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	970	10/2000
<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>	ID	10/2000
<b>Aquatic maximum value (AMV)</b>	ID	10/2000
<b>Final Acute Value (FAV)</b>	ID	10/2000

Sources:

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



**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	50	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	5	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	1.30E+01	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	4.50E+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