



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Tetranitromethane
CAS #:	509-14-8
Revised By:	RRD Toxicology Unit
Revision Date:	November 30, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	196.03	196.03	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	13.8	13.80	EPI	EXP
Boiling Point (°C)	259	126.10	EPI	EXP
Solubility (ug/L)	85000	900000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	8.42	8.42E+00	EPI	EXP
HLC (atm-m³/mol at 25°C)	2.60E-5	2.40E-04	PP	EST
Log Kow (log P; octanol-water)	-2.05	-2.05	PP	EST
Koc (organic carbon; L/Kg)	9.66E-3	428.3	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.08	3.35E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.0E-6	8.60E-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	NA	NA	NA
Lower Explosivity Level (LEL; unitless)	NA	NA	NA	NA
Critical Temperature (K)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		9.74E+03	CRC	EXP
Density (g/mL, g/cm ³)		1.638	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.75E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	2.15E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	2.44E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	2.73E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	--	NA	MDEQ, 2015	
RfD details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS file is available at this time. PPRTV: No PPRTV record is available at this time. MRL: No MRL record is available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day) ⁻¹)	--	NA	MDEQ, 2015	
CSF details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS file is available at this time. PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m ³)	--	4.0E-1	MDEQ, 2000	
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS file is available at this time. PPRTV: No PPRTV record is available at this time. MRL: No MRL record is available at this time.</p> <p>Tier 3 Sources: MDEQ Basis: For the initial threshold screening level (ITSL) screening level development, the ACGIH TLV (0.005 ppm) value provides the best basis for</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>screening level development. It is the most recently developed OEL, and considers the latest toxicity information. The ITSL is most appropriately based on the ACGIH TLV of 0.005 ppm [or 40 micrograms per cubic meter ($\mu\text{g}/\text{m}^3$)]. According to R232(c), determining the ITSL from the OEL, the ITSL is equivalent to 1/100 of the OEL. Therefore, the ITSL is being established as $0.4 \mu\text{g}/\text{m}^3$ with an 8-hour averaging time.</p> <p>Source and date: MDEQ-CCD/AQD and Tetranitromethane AQD File, 12/04/2000</p> <p>California OEHHA 2002: No significant risk level (NSRL) = $0.059 \mu\text{g}/\text{day}$. Derived from a human inhalation cancer potency estimate = $12 (\text{mg}/\text{kg}/\text{day})^{-1}$ in male mice. Cancer study information is as follows:</p> <p>Critical Study: National Toxicology Program (NTP, 1990). Toxicology and Carcinogenesis Studies of Tetranitromethane in F344 Rats and B6C3F1 Mice (Inhalation Studies). Technical Report Series No. 386. NIH Publication No. 90-2841. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health.</p> <p>Methods: Groups of 50 male and 50 female B6C3F1 mice were exposed via inhalation to tetranitromethane six hours per day, five days per week at 0, 0.5 or 2 ppm for 103 weeks.</p> <ol style="list-style-type: none"> 1) <i>Dose response data: Tumor Type</i> – alveolar/bronchiolar carcinomas/adenomas and squamous cell carcinomas of the lung; <i>Test Species</i> - B6C3F₁ male mouse; <i>Route</i> - inhalation 2) <i>Extrapolation method:</i> multistage polynomial model <p>Source and date: No significant risk level (NSRL) for the proposition 65 carcinogen tetranitromethane. Reproductive and Cancer Hazard Assessment Section, Office of Environmental Health Hazard Assessment (OEHHA), California Environmental Protection Agency. August 2002.</p> <p>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, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹)	--	1.5E-2	MDEQ, 2000	
IURF details	NA	<p>Basis: MDEQ is selected because the MDEQ IURF is in the appropriate units (($\mu\text{g}/\text{m}^3$)⁻¹) while the CAL IURF is presented in units of (mg/kg/day)⁻¹. The same study is used by both agencies and AQD documentation is available.</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: NA WOE Basis: NA</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file is available at this time. PPRTV: No PPRTV record is available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: IURF = 1.5E-2 ($\mu\text{g}/\text{m}^3$)⁻¹ (2000). Critical Study: National Toxicology Program (NTP, 1990). Toxicology and Carcinogenesis Studies of Tetranitromethane in F344 Rats and B6C3F1 Mice (Inhalation Studies). Technical Report Series No. 386. NIH Publication No. 90-2841. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health. Method(s): The 1990 NTP 2-year inhalation study found increased incidences of lung tumors in both sexes of rats and mice. Male mice lung adenoma and carcinoma incidence of 12/50, 27/47 and 47/48 in the control, 0.71 and 2.9 mg/m³ daily dose groups was used to calculate the slope factor. 3) <i>Dose response data: Tumor Type</i> – lung adenoma and carcinomas ; <i>Test Species</i> - Male mouse; <i>Route</i> - inhalation 4) <i>Extrapolation method:</i></p> <p>Source and Date: MDEQ-AQD, 12/4/2000.</p> <p>California OEHHA 2002: human cancer potency <u>estimate</u> = 12 (mg/kg/day)⁻¹. Value not listed in Cal OEHHA toxicity criteria database.</p>	Complete	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Critical Study: National Toxicology Program (NTP, 1990). Toxicology and Carcinogenesis Studies of Tetranitromethane in F344 Rats and B6C3F1 Mice (Inhalation Studies). Technical Report Series No. 386. NIH Publication No. 90-2841. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health.</p> <p>Methods: Groups of 50 male and 50 female B6C3F1 mice were exposed via inhalation to tetranitromethane six hours per day, five days per week at 0, 0.5 or 2 ppm for 103 weeks.</p> <p>5) <i>Dose response data: Tumor Type</i> – alveolar/bronchiolar carcinomas/adenomas and squamous cell carcinomas of the lung; <i>Test Species</i> - B6C3F₁ male mouse; <i>Route</i> - inhalation</p> <p>6) <i>Extrapolation method:</i> multistage polynomial model</p> <p>Source and date: No significant risk level (NSRL) for the proposition 65 carcinogen tetranitromethane. Reproductive and Cancer Hazard Assessment Section, Office of Environmental Health Hazard Assessment (OEHHA), California Environmental Protection Agency. August 2002.</p> <p>Other Tier 3: 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 (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
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, 2014	
Developmental or Reproductive Toxicity Details	NA	NA		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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 (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)	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 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 (AE _d)	---	0.1	MDEQ, 2015	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		1.0	MDEQ, 2015	
AE _i 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) Analytical Information

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	500	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	100	MDEQ, 2015
Target Detection Limit – Air (ppbv)	2.10E-04	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	7.10E-03	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