



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>2,2,4-Trimethyl pentane</b>
<b>CAS #:</b>	<b>540-84-1</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 16, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	114.23	114.23	EPI	EXP
<b>Physical State at ambient temp</b>	Liquid	Liquid	MDEQ	
<b>Melting Point (°C)</b>	-107.5	-107.30	EPI	EXP
<b>Boiling Point (°C)</b>	99.24	99.20	EPI	EXP
<b>Solubility (ug/L)</b>	2330	2440	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	46.89	4.93E+01	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	3.13E+0	3.03E+00	CRC	EXP
<b>Log Kow (log P; octanol-water)</b>	4.09	1.09	PP	EST
<b>Koc (organic carbon; L/Kg)</b>	2080	240.3	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	5.74E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	7.06E-06	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
Flash Point (°C)	10 F	-12	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.011	0.011	PC	EXP
Critical Temperature (K)		543.9	CRC	EXP
Enthalpy of Vaporization (cal/mol)		7.36E+03	CRC	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.6878	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.70E-05	2.81E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	6.61E-05	6.92E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	3.85E-05	4.49E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	9.38E-05	1.10E-04	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><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (7/31/2007), no value at this time. An IRIS Toxicological Review is available.  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day <sup>-1</sup> )	--	NA	MDEQ, 2015	
CSF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "inadequate information to assess carcinogenic potential" for 2,2,4-trimethylpentane  <b>IRIS WOE Basis:</b> No chronic bioassay studies are available. The few studies available on its genotoxic potential were negative.  <b>Source and Date:</b> IRIS, Last revision date - 7/31/2007</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (7/31/2007), no value at this time.  <b>PPRTV:</b> No PPRTV record available 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
Reference Concentration (RfC) or Initial Threshold	3.5E+3	3.5E+3	MDEQ, 2005	



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
<b>Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>				
<b>RfC/ITSL details</b>	<p>Chronic RfC: 8 hr. averaging time. Based on NIOSH REL = 350 mg/m<sup>3</sup>. Rule 232(1) (c). CCD/AQD, 3/08/2005</p>	<p><b>Tier 3 Source:</b> <b>MDEQ:</b> <b>Basis:</b> MDEQ ITSL based on 1977 NIOSH REL for C5-8 alkanes. ECHA REACH derived a value for 2,2,4-trimethylpentane based on an inhalation study of nonane (CAS # 111-84-2). See details below.</p> <p><b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (7/31/2007), no value at this time. An IRIS Toxicological Review is available. <b>PPRTV:</b> No PPRTV record available at this time. <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Sources:</b> <b>MDEQ/AQD (03/08/2005):</b> AQD ITSL = 3.5E+3 <math>\mu\text{g}/\text{m}^3</math> with 8 hr. averaging time. Basis: 1977 NIOSH REL 350 mg/m<sup>3</sup> for neurotoxicity of C5-8 alkanes. The ACGIH has a TLV of 300 ppm (1400 mg/m<sup>3</sup>) for all isomers of octane for prevention of narcosis effects. The REL for C5-8 alkanes includes most forms of octane including isooctane (2,2,4-trimethylpentane). NIOSH indicated that workers are usually exposed to mixtures containing many different alkanes. Reference: NIOSH. 1977. Criteria for a recommended standard...occupational exposures to alkanes (C5-8). DHEW 77-151. Source and date: MDEQ-CCD/AQD, 3/08/2005</p> <p><b>ECHA (REACH):</b> Derived No Effect Level (DNEL) = 608 mg/m<sup>3</sup> (6.1E+5 <math>\mu\text{g}/\text{m}^3</math>) Basis: Guideline: OECD Guideline 413 (Subchronic Inhalation Toxicity: 90-Day) Key study: Carpenter, C.P. et al. 1978. Petroleum hydrocarbon toxicity studies XVII. Animal response to n-nonane (CAS # 111-84-2) vapor. Toxicology and Applied Pharmacology 44: 53-61. Method: male Harlan-Wistar rats (25/dose) were exposed to 0, 1.9, 3.1, 8.4 mg/L (corresponding to 360, 590, 1600 ppm) by inhalation (vapor) for 6 hrs./day, 5</p>		Complete



	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
		<p>days/wk. for 13 weeks.  Dose descriptor starting point: NOAEC – 8.4 mg/L (8400 mg/m<sup>3</sup> air)  Critical effect: clinical signs and decreased body weight  Overall assessment factor (AF): 10 (details not specified)  Source: ECHA REACH Dossier on 2,2,4-Trimethyl Pentane</p> <p><b>Other Tier 3:</b> 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) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) (( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup> )	--	NA	MDEQ, 2015	
IURF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> "inadequate information to assess carcinogenic potential" for 2,2,4-trimethylpentane  <b>IRIS WOE Basis:</b> No chronic bioassay studies are available. The few studies available on its genotoxic potential were negative.  <b>Source and Date:</b> IRIS, Last revision date - 7/31/2007</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (7/31/2007), no value at this time.  <b>PPRTV:</b> No PPRTV record available 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
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		

	Part 201 Value	Updated Value	Source*/Reference /Date	Comments/Notes /Issues
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)	--	NA	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (ug/L)	--	NA	SDWA, 1976 and USEPA SMCL List, 2015	
SMCL details	NA	NA		
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 (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E	
ABS <sub>gi</sub> details		RAGS E (EPA, 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>	NA
<b>Updated GSI value (µg/L)</b>	NA
<b>Rule 57 Drinking Water Value (µg/L)</b>	NA

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>		
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>		
<b>Wildlife Value (WV)</b>		
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>		
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>		
<b>Final Chronic Value (FCV)</b>		
<b>Aquatic maximum value (AMV)</b>		
<b>Final Acute Value (FAV)</b>		

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>	2,500	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	50	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	7.40E+02	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	2.50E+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