



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Methylcyclopentane</b>
<b>CAS #:</b>	<b>96-37-7</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 16, 2105

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	84.16	84.16	EPI	EXP
<b>Physical State at ambient temp</b>	Liquid	Liquid	MDEQ	
<b>Melting Point (°C)</b>	---	-142.50	EPI	EXP
<b>Boiling Point (°C)</b>	71.8	71.80	EPI	EXP
<b>Solubility (ug/L)</b>	73890	42000	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	137.84	1.38E+02	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	3.63E-1	3.62E-01	CRC	EXP
<b>Log Kow (log P; octanol-water)</b>	3.37	3.37	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	2060	128.3	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	7.88E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	8.93E-06	W9	EST
<b>Soil Water Partition Coefficient (Kd; inorganics)</b>	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	NA	-29	CRC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.01	CRC	EXP
Critical Temperature (K)		532.78	CRC	EXP
Enthalpy of Vaporization (cal/mol)		6.95E+03	CRC	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.7486	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	2.66E-05	2.81E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	6.34E-05	6.93E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	3.77E-05	4.49E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	8.91E-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	NA	MDEQ, 2015	
RfD details	--	<p><b>Basis:</b> EPA/NCEA does not support the extrapolation of the subchronic p-RfD to a chronic p-RfD (see discussion below); therefore, no RfD value for methylcyclopentane is available at this time.</p> <p><b>Tier 1 Source:</b>  <b>IRIS:</b> No IRIS file available for methylcyclopentane at this time.</p> <p><b>Tier 2 Sources:</b>  <b>PPRTV (09/15/2009):</b> Subchronic p-RfD = 4E-1 mg/kg/d.  <b>Critical Study:</b> Halder, C.A., et al. (1985). Hydrocarbon nephropathy in male rats: Identification of the nephrotoxic components of unleaded gasoline. Toxicol. Ind. Health. 1:67–87.  <b>Method:</b> Groups of 10 male Fischer 344 rats were administered 500 or 2,000 mg/kg of undiluted methylcyclopentane (98% purity) by gavage, once daily, 5 days/week for 4 weeks. A negative control group received isotonic saline at a dose of 2,000 mg/kg/day.  <b>Critical effect:</b> Reduction in body weight gain.  <b>End point or Point of Departure (POD):</b> The reduction in body weight gain at the low dose was considered to be minimal therefore the low dose was considered a NOAEL. The NOAEL was first adjusted to continuous exposure from the 5 days/week dosing schedule. The NOAEL<sub>ADJ</sub> was calculated as the study NOAEL x 5/7 (500 x 5/7 = 357 mg/kg-day).  <b>Uncertainty Factors:</b> UF = 1,000 (10 for inter-species extrapolation; 10 for intra-species differences; 10 for database uncertainty as only 2 sub chronic studies are available and no developmental or multigenerational reproduction studies are available).  <b>Per EPA/NCEA:</b> The studies by Borriston Laboratories (1985; Halder et al., 1985) are considered inappropriate for deriving a chronic RfD because of the short duration of the dosing regimens. Additionally, based on data from Ono et al.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		(1981) and Krasavage et al. (1980), the overt neurological endpoint identified in Ono et al. may require significantly more than 4 weeks of exposure before it becomes apparent in rodents. Thus, extension of the sub chronic results to chronic exposures (even with an additional uncertainty factor) may not be warranted.  <b>MRL:</b> No MRL record for methylcyclopentane is available at this time.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no oral toxicity endpoint reported by DEQ (a lit search was conducted in June, 1992 – data inadequate for criteria development).		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	NA	NA	MDEQ, 2015	
<b>CSF details</b>	--	<b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> No IRIS file available for methylcyclopentane at this time. <b>PPRTV (09/15/2009):</b> Inadequate information to assess the carcinogenic potential of methylcyclopentane. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no oral toxicity endpoint reported by DEQ.		Complete
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)</b>	NA	7.0E+2	MDEQ, 2010	
<b>RfC/ITSL details</b>	--	<b>Tier 3 Source:</b> <b>MDEQ:</b> <b>Basis:</b> The Tier 3 MDEQ value is preferred because it is based on the new IRIS value for the surrogate, n-hexane. MADEP used the 1993 IRIS RfC for n-hexane. See details below.		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file for methylcyclopentane is available at this time.  <b>PPRTV (09/15/2009):</b> Per PPRTV, there is inadequate information available to develop an inhalation toxicity value at this time.  <b>MRL:</b> No MRL record for methylcyclopentane is available at this time.</p> <p><b>Tier 3 Sources:</b>  <b>MDEQ/AQD (10/04/2010):</b> Per DEQ-CCD, AQD ITSL = 7E+2 µg/m<sup>3</sup>: A comparison to other C6 (six carbon) chemicals, finds n-hexane RfC based ITSL is the lowest. As there is no adequate toxicity data on pure methylcyclopentane it is considered appropriate to utilize the lowest other ITSL as the basis for the methylcyclopentane ITSL. The n-hexane RfC value is based on the 12/23/2005 IRIS value.</p> <p><b>Massachusetts DEP (2003):</b> RfC= 0.2 mg/m<sup>3</sup> (2.0E+2 µg/m<sup>3</sup>) based on the U.S. EPA (1993a) derived RfC of 0.2 mg/m<sup>3</sup> for n-hexane, which is based on a neurotoxic endpoint, as a representative surrogate for the C5-C8 fraction. The updated IRIS (12/23/2005) n-hexane RfC is 7.0E+2 µg/m<sup>3</sup>.</p> <p><b>Texas CEQ:</b> RfC = 1.0E+0 mg/m<sup>3</sup> (1.0E+3 µg/m<sup>3</sup>).</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, Minnesota, New Jersey and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m <sup>3</sup> ) <sup>-1</sup> )	NA	NA	MDEQ, 2015	
IURF details	--	<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file for methylcyclopentane is available at this time.  <b>PPRTV (09/15/2009):</b> Per PPRTV, a provisional inhalation unit risk could be derived for methylcyclopentane because of the lack of suitable human or animal,</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		oral or inhalation data. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no inhalation toxicity value for methylcyclopentane is available at this time.		
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	No	USEPA, 2015	
<b>MMOA Details</b>	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List		
<b>Developmental or Reproductive Effector? (Y/N)</b>	--	No	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	--	The RfC is not based on a reproductive-developmental effect.		
<b>State Drinking Water Standard (SDWS) (µg/L)</b>	--	NO	SDWA, 1976	
<b>SDWS details</b>	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (µg/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
--	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
<b>Is there an Aesthetic Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Aesthetic value details</b>	NA	NA		
<b>Is there a Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
<b>Phytotoxicity details</b>	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>	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>	2.02E+04	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	6.72E+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 OEHHHA	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