



CHEMICAL UPDATE WORKSHEET

Chemical Name:	N-methylaniline
CAS #:	100-61-8
Revised By:	RRD Toxicology Unit
Revision Date:	August 19, 2105

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	107.15	107.16	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	-57	-57.00	EPI	EXP
Boiling Point (°C)	384.6	196.20	EPI	EXP
Solubility (ug/L)	5.62E+6	5620000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.453	4.53E-01	EPI	EXP
HLC (atm-m³/mol at 25°C)	8.88E-6	8.88E-06	EPI	EXP
Log Kow (log P; octanol-water)	1.66	1.66	EPI	EXP
Koc (organic carbon; L/Kg)	43	82.08	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.08	7.21E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.0E-6	9.13E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	174.9	79.4	NPG	EXP
Lower Explosivity Level (LEL; unitless)	NA	NA	NA	NA
Critical Temperature (K)		702	CRC	EXP
Enthalpy of Vaporization (cal/mol)		1.27E+04	HSDB	EXP
Density (g/mL, g/cm ³)		0.9891	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	9.47E-06	1.24E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	9.56E-06	1.30E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	1.14E-05	1.62E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	1.14E-05	1.64E-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	2.0E-3	PPRTV, 2005	
RfD details	New Hazardous Substance	<p>Tier 2 Source: PPRTV: Basis: PPRTV is a Tier 2 source, no Tier 1 available PPRTV chronic RfD = 2E3 mg/kg-day. Critical Study: GINC (Global Information Network on Chemicals). 2003. N-Methylaniline. CAS No. 100-61-8. Summary of Toxicity Data. (Eng.). Chemical Toxicity Database. Ministry of Health, Labor and Welfare, Japan. Online. http://wwwdb.mhlw.go.jp/ginc/dbfile1/file/file100-61-8.html Method: Rats were exposed to n-methylaniline by gavage for 28 days. Doses of 0, 5, 25 or 125 mg/kg-day were administered by gavage in corn oil to groups of CD rats (5/sex) for 28 days. Hematology, urinalysis and clinical chemistry data were collected before terminal sacrifice on day 29. The liver, kidney, spleen, bone marrow, adrenal and femur were evaluated for histopathology. Critical effect: Minimal effects on erythrocytes (significantly reduced hemoglobin in females) and slight congestion of the spleen in males were observed at the NOAEL of 5 mg/kg-day. At the LOAEL of 25 mg/kg-day, significant evidence of anemia (reduced hematocrit, hemoglobin and erythrocyte counts), as well as compensatory hematopopiesis was observed in both sexes. Pigment deposition in several tissues at 125 mg/kg-day was presumably related to erythrocyte destruction. End point or Point of Departure (POD): NOAEL = 5 mg/kg-day and LOAEL = 25 mg/kg-day. Chronic RfD = 2E-3 mg/kg-day (5 mg/kg-day divided by an UF of 3000). Uncertainty Factors: UF = 3,000: 10 for extrapolation from rats to humans, 10 to protect sensitive individuals, and 3 for database deficiencies including the absence of supporting chronic to subchronic studies and any reproduction or developmental studies and 10 for use of a subchronic study. Confidence in the critical study is low. The study included investigation of a broad array of systemic endpoints in multiple dose groups and identified a NOAEL and LOAEL. Tabular</p>		COMPLETE

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>results were well reported. The study was limited by small group sizes, short duration, and failure to analyze for methemoglobin. Confidence in the database is low because of the lack of supporting systemic toxicity data and developmental and reproductive toxicity studies. Confidence in the subchronic and chronic p-RfDs for N-methylaniline is, therefore, low.</p> <p>Source and date: PPRTV, 08/03/2005</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD-SWQD (06/21/2006), insufficient data were available to derive human health values. No values reported by RRD however, an evaluation was conducted and it was determined that data were insufficient to derive toxicity endpoints (December 2008). The study cited and used in development of the p-RfDs (PPRTV) was not identified in the RRD Tox Assessment.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day⁻¹)	NA	NA	MDEQ, 2015	
CSF details	New Hazardous Substance	<p>Tier 1 and 2 Sources IRIS: No IRIS file available at this time. PPRTV: No cancer data available for the PPRTV evaluation dated 08/03/2005. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD-SWQD (06/21/2006), insufficient data were available to derive human health values. No values reported by RRD however, an evaluation was conducted and it was determined that data were insufficient to derive toxicity endpoints.</p>		COMPLETE
Reference Concentration (RfC) or Initial	NA	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)				
RfC/ITSL details	New Hazardous Substance	Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (08/03/2005), no inhalation data reported or evaluated. MRL: No MRL record available at this time. Tier 3 Source: MDEQ: Per DEQ-CCD, no information reported by AQD.		COMPLETE
Inhalation Unit Risk Factor (IURF) ($(\mu\text{g}/\text{m}^3)^{-1}$)	NA	NA	MDEQ, 2015	
IURF details	New Hazardous Substance	Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (08/03/2005), no inhalation data reported or evaluated. MRL: NA; MRLs are for non-cancer effects only – no record available. Tier 3 Source: MDEQ: Per DEQ-CCD, no information reported by AQD.		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		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) ($\mu\text{g}/\text{L}$)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Secondary Maximum Contaminant Level (SMCL) (µg/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? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	NA		
Others:				

(C) Chemical-specific Absorption 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)	---	NA	MDEQ, 2015	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		NA	MDEQ, 2015	
AE _i Details				
Relative Source Contribution for Water (RSC _w)		NA	MDEQ, 2015	
Relative Source Contribution for Soil (RSC _s)		NA	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)	ID
Updated GSI value (µg/L)	ID
Rule 57 Drinking Water Value (µg/L)	ID

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	ID	7/2006
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	ID	7/2006
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	NA
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	NA
Final Chronic Value (FCV)	ID	7/2006
Aquatic maximum value (AMV)	ID	7/2006
Final Acute Value (FAV)	ID	7/2006

Sources:

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



(E) Target Detection Limits (TDL)

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	330	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	1	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