



CHEMICAL UPDATE WORKSHEET

Chemical Name:	n-Nitrosodiphenylamine
CAS #:	86-30-6
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)	198.22	198.23	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	340	66.50	EPI	EXP
Boiling Point (°C)	---	101.00	PC	EXP
Solubility (ug/L)	35100	35000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.0988	1.00E-01	PP	EST
HLC (atm-m ³ /mol at 25°C)	5.00E-6	5.00E-06	SSG	EXP
Log Kow (log P; octanol-water)	3.16	3.13	EPI	EXP
Koc (organic carbon; L/Kg)	381	2632	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.0312	2.84E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	6.35E-6	7.19E-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)		890.45	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		7.30E+03	EPA2001	EST
Density (g/mL, g/cm ³)		1.23	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	1.17E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	1.17E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	1.48E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	1.48E-06	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	2.5E-1	2.5E-1	MDEQ, 1989	
RfD details	Per EPB, DEQ/SWQD (12/1/1989): LOAEL (weight depression and corneal opacity) of 1,000 ppm (50 mg/kg/d) in male and female F344 rats exposed via feed for 100 weeks (UF=200; 2 x for minimal effects) (NCI, 1979). Per EPB, RRD (12/1/1989): IRIS data file empty. (i.e. No noncancer data in IRIS.)	<p>Tier 3 Source: MDEQ: Basis: No other values were returned in the Tier 3 search. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (07/01/1993), no value at this time. PPRTV: Per PPRTV (9/19/2007), NA: the poor quality of the available data, the availability of an IRIS oral slope factor addressing the cancer and hyperplasia risk observed in rats, and major uncertainties in dosing and modeling results led us to conclude that data were insufficient to derive either a chronic or a subchronic p-RfD for N-nitrosodiphenylamine. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD-SWQD, 12/1/1989. RfD = 0.25 mg/kg/day; LOAEL (weight depression and corneal opacity) of 1000 ppm (50 mg/kg/day) in male and female F344 rats exposed via feed for 100 weeks (UR = 200; 2 x for minimal effects) NCI, 1979.</p> <p>Other Tier 3: No value is available from these sources/databases: HEAST, NTP ROC, California OEHHA, Massachusetts DEP 2015, Minnesota 2015, New Jersey 2008, New York 2006, Texas CEQ 2014, WHO (IARC and IPCS/INCHEM), Canada 2010, RIVM, ECHA (REACH), OECD HPV.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	3.1E-3	4.9E-3	IRIS, 1993	
CSF details	Per EPB, DEQ/SWQD (12/1/1989): LOAEL (weight	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. Critical Study: NCI (National Cancer Institute). 1979. Bioassay of N-</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	depression and corneal opacity) of 1,000 ppm (50 mg/kg/d) in male and female F344 rats exposed via feed for 100 weeks (UF=200; 2 x for minimal effects) (NCI, 1979). Per EPB, RRD (12/1/1989): IRIS data file empty. (i.e. No noncancer data in IRIS.)	<p>Nitrosodiphenylamine for Possible Carcinogenicity. NCI Carcinogenesis Technical Report Series No. 164. NIH 79-1720. NTIS PB 298-275.</p> <p>Methods: N-nitrosodiphenylamine (98% pure containing two unspecified impurities) was administered at 0, 1000 or 4000 ppm in diet to groups of 50 F344 rats/ sex. Matched controls consisted of 20 rats/sex. Tumor Type: transitional cell carcinoma of the bladder. Extrapolation method = Linearized multistage procedure, extra risk.</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probably human carcinogen</p> <p>IRIS WOE Basis: Increased incidence of bladder tumors in male and female rats and reticulum cell sarcomas in mice, and structural relationship to carcinogenic nitrosamines.</p> <p>Source: IRIS, 7/1/1993</p> <p>Tier 2 Sources:</p> <p>PPRTV: Per PPRTV, 9/19/2007: IRIS (U.S. EPA, 1993) reported an oral slope factor of 4.9×10^{-3} per mg/kg-day, based on transitional cell carcinomas of the bladder in female F344 rats reported by NCI (1979).</p> <p>MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source:</p> <p>MDEQ: Per DEQ-CCD-RRD, 9/13/1999, CSF = 0.0031 per mg/kg/day. B2 carcinogen; transitional cell carcinoma of the bladder in female rats; drinking water study (NCI, 1979). IRIS SF revised with new species scaling factor.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	--	NA	MDEQ, 2015	
RfC/ITSL details	--	<p>Tier 1 and 2 Sources:</p> <p>IRIS: Per IRIS (7/1/1993), no value at this time.</p> <p>PPRTV: Per PPRTV (9/19/2007), a provisional inhalation RfC could not be derived for N-nitrosodiphenylamine because data on adverse health effects following</p>		Complete.

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		inhalation exposure were lacking for humans and animals. Without pharmacokinetic data and information to rule out portal-of-entry effects, there was no basis to support a route-to-route extrapolation from the oral data, even if it were otherwise considered sufficient. MRL: No MRL record available at this time. Tier 3: MDEQ: No DEQ record available at this time.		
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$)⁻¹)	--	NA	MDEQ, 2015	
IURF details	--	Tier 1 and 2 Sources: IRIS: Per IRIS (7/1/1993), no value at this time. PPRTV: Per PPRTV (9/19/2007), no quantitative estimate of cancer risk from inhalation exposure was available on IRIS. None was developed here due to lack of information. MRL: NA; MRLs are for non-cancer effects only. Tier 3 Source: MDEQ: No DEQ record available at this time.		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	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
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 (A _{Ed})	---	0.1	MDEQ, 2015	
A _{Ed} details				
Ingestion Absorption Efficiency (A _{Ei})		1.0	MDEQ, 2015	
A _{Ei} 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) Target Detection Limits (TDL)

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	330	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	5	MDEQ, 2015
Target Detection Limit – Air (ppbv)	NA	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	NA	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

