



CHEMICAL UPDATE WORKSHEET

Chemical Name:	n-Nitrosodinpropylamine
CAS #:	621-64-7
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	130.22	130.19	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	---	NA	NA	NA
Boiling Point (°C)	206	206.00	EPI	EXP
Solubility (ug/L)	9.89E+6	13000000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	3.496	8.60E-02	PP	EST
HLC (atm-m³/mol at 25°C)	2.25E-6	5.38E-06	EPI	EXP
Log Kow (log P; octanol-water)	1.4	1.36	EPI	EXP
Koc (organic carbon; L/Kg)	23.8	275.4	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.0545	5.64E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.17E-6	7.76E-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)		746.87	EPA2001	EXP
Enthalpy of Vaporization (cal/mol)		6.10E+03	EPA2001	EST
Density (g/mL, g/cm ³)		0.9163	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	5.05E-06	5.17E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	5.05E-06	5.17E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	6.04E-06	6.54E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	6.04E-06	6.54E-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	NA	MDEQ, 2015	
RfD details	12/1/89: DEQ/SWQD; (Oral, SWQD): LOAEL (weight depression and corneal opacity) of 1000 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). Empty IRIS file date.	<p>Basis: The available toxicity data are inadequate for the development of a chronic RfD.</p> <p>Tier 1 Source: IRIS (03/31/1987): Per IRIS, no RfD is available at this time.</p> <p>Tier 2 Sources: PPRTV: No PPRTV record available at this time. MRL (12/1989): Per ATSDR, oral acute MRL = 0.095 mg/kg/day Critical Study: Tyndall RL, Clapp NK, Davidson KA, et al. (1978) Effects of carcinogenic and non-carcinogenic chemicals on plasma esterases in BALB/C mice. Chem Biol Interactions 23:159-169. Methods: mice exposed to 9.5 mg/kg/day via drinking water for one week End point or Point of Departure (POD): NOAEL = 9.5 mg/kg/day Critical effect: hepatic effects Uncertainty Factors: UF = 100 (10 each for intra- and interspecies variability) Source and date: ATSDR final 12/1989</p> <p>Tier 3 Source: MDEQ/RRD: Per DEQ-CCD, RRD references a WRD-developed RfD; however, WRD reports no RfD value for this chemical.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	4.5E+0	7.0E+0	IRIS, 1993	
CSF details	3/15/2000 IRIS; Hepatocellular carcinomas in rats administered NDPA in drinking water (Druckery,	<p>Tier 1 Source: IRIS: Basis: The IRIS and RRD values are based on the same study data and differ only in the species scaling factor applied. The IRIS value is selected consistent with the toxicity value decision framework order of source preference.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	<p>1967; Druckery et al., 1967); Oral SF calculated in IRIS using the "one-hit model". EPA IRIS oral SF was adjusted by multiplying the animal slope factor by the ratio of the human body weight to animal body weight (0.35 - rats) rose to the 1/4 power. EPA Classification: B2 carcinogen.</p>	<p>Tier 1 Source: IRIS (07/01/1993): oral slope factor = 7.0E+0 per mg/kg/d. Critical Studies: 1) Druckrey, H., R. Preussmann, S. Ivankovic and D. Schmahl. (1967). Organotropism carcinogenic activities of 65 different N-Nitroso compounds in BD-rats. Z. Krebsforsch. 69(2): 103-201. 2) Druckrey, H. (1967). Quantitative aspects in chemical carcinogens. In: Potential Carcinogenic Hazards from Drugs, Evaluation of Risks, R. Truhart, Ed. UICC Monograph, Series 7. Berlin Springer-Verlag. p. 60-78. Methods: As part of a survey of 65 N-nitroso compounds, Druckrey et al. (1967) administered N-nitrosodi-n-propylamine in drinking water to BD rats of unspecified sex. A total of 48 rats was treated in groups inferred to number 16, 16, 15 and 1 at doses of 4, 8, 15 or 30 mg/kg/day, respectively, for life. <i>Extrapolation Method:</i> One-hit Carcinogen Weight-of-Evidence (WOE) Class: B2; probably human carcinogen. IRIS WOE Basis: Increased tumor incidence at multiple sites in two rodent species and in monkeys administered the compound by various routes. Source and date: IRIS, 7/1/1993</p> <p>Tier 2 Sources: PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ/RRD (3/15/2000): Per DEQ-CCD, oral CSF = 4.5 per mg/kg/day. Basis: Hepatocellular carcinomas in rats administered N-nitroso-di-n-propylamine in drinking water (Druckery, 1967; Druckery et al., 1967); EPA's oral SF was calculated by IRIS using the "one-hit model" and by applying a 1/3 power body weight scaling factor. MDEQ applied a 1/4 power body weight scaling factor per the current EPA cancer guidelines.</p>		
Reference Concentration	NA	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
(RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)				
RfC/ITSL details	--	<p>Tier 1 and 2 Sources: IRIS (03/31/1987): Per IRIS, no RfC value available at this time. PPRTV: No PPRTV record available at this time. MRL (12/1989): Per ATSDR, no inhalation MRL available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Inhalation Unit Risk Factor (IURF) ($(\mu\text{g}/\text{m}^3)^{-1}$)	2.0E-3	2.0E-3	MDEQ, 1995	
IURF details	(Air, AQD): Inhalation potency was derived by converting EPA's oral potency listed in IRIS. EPA's oral potency based on hepatocellular carcinomas in BD rats following drinking water exposure reported by Druckrey et al 1967, Druckrey 1967. 8/22/1995.	<p>Tier 3 Source: MDEQ: Basis: AQD's value is identical to CalEPA's, both of which are based on the same extrapolation method from the EPA oral slope factor value. Therefore, the AQD value is selected. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (07/01/1993), no value at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ/AQD (8/22/1995): Per DEQ-CCD, IURF = 0.002 per $\mu\text{g}/\text{m}^3$. AT = annual. Inhalation potency was derived by converting EPA's oral potency listed in IRIS. EPA's oral potency based on hepatocellular carcinomas in BD rats following drinking water exposure reported by Druckrey, et al. (1967) and Druckrey, (1967).</p> <p>California DTSC: IURF= 0.002 ($\mu\text{g}/\text{m}^3$)⁻¹ derived from extrapolation of HEAST (1986) oral slope factor of 7.0 per mg/kg/d, assuming 20 m³/day human breathing</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>rate and 70 kg body weight.</p> <p>Minnesota PCA: IUR= 2.00E-3 ($\mu\text{g}/\text{m}^3$)⁻¹ based on CalEPA.</p> <p>New Jersey: URF= 2.0E-3 ($\mu\text{g}/\text{m}^3$)⁻¹ based on CalEPA.</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, 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	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List		
Developmental or Reproductive Effector? (Y/N)	--	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	--	NA		
State Drinking Water Standard (SDWS) ($\mu\text{g}/\text{L}$)	NA	NO	SDWA, 1976	
SDWS details	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) ($\mu\text{g}/\text{L}$)	NA	NO	SDWA, 1976 and USEPA SMCL List	
SMCL details	--	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	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	---	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) 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 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